BIOSYSTEMS AND FOOD ENGINEERING

RESEARCH REVIEW 23

UCD SCHOOL OF BIOSYSTEMS AND FOOD ENGINEERING

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Document Number: ISSN 1649-475X

May 2018

Editors: Enda J. Cummins and Thomas P. Curran

FOREWORD

The Twenty Third Annual **Research Review** describes the ongoing research programme in the School of Biosystems and Food Engineering at University College Dublin from over 98 researchers (12 academic staff, 1 technician, 11 postdoctoral researchers and 74 postgraduates). The research programme covers three focal areas: Food and Process Engineering; Bioresource Systems; and Bioenvironmental Engineering. Each area is divided into sub-areas as outlined in the Table of Contents which also includes the name of the research scholar (in bold); the research supervisor(s); the title of the research; the nature of the research programme; and the research sponsors. It also includes the noting of four awards for presentational excellence at the Twenty First Annual **Biosystems and Food Engineering Research Seminar** held in University College Dublin on **Tuesday 20th March 2018**.

The six Appendices in the Review provide:

- a listing of research projects in progress which were not included in the Review;
- profiles of Postdoctoral Research Scholars;
- links to Postgrad Research Activities with YouTube Videos

The Editors gratefully acknowledge the dedicated work of the individual research scholars, their research supervisors and the financial support of research sponsors. Suggestions as to how future editions might be improved in presentation, style or content would be greatly appreciated. A copy of this book is available to download from the UCD Research Repository at: **http://researchrepository.ucd.ie**

The review also includes papers from the School's Taught Masters Programmes as follows:

ME - Biosystems and Food Engineering
http://www.ucd.ie/eacollege/studywithus/engineering/biosystemsfood/biosystems.html

MEngSc – Food Engineering
http://www.ucd.ie/eacollege/studywithus/engineering/biosystemsfood/food.html

MSc – Environmental Technology
http://www.ucd.ie/eacollege/studywithus/engineering/biosystemsfood/environmental.html

MSc – Sustainable Energy and Green Technologies
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ENDA CUMMINS and TOM CURRAN 31st May 2018

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APPENDICES

*MEngSc Res = Research Masters (Mode 1)

INITIAL ASSESMENT OF RAMAN HYPERSPECTRAL IMAGING USING POINT MAPPING AND STREAMLINE IMAGING

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Abstract
Raman hyperspectral imaging has potential as a diagnostic tool through the identification of anomalies in the chemical makeup of biological samples. This is done through the measurement of minute changes in the energy of reflected photons, known as Stokes and anti-Stokes scattering. This preliminary investigation examines the necessary preparatory steps for the imaging of the tissue and the effectiveness of point mapping and streamline imaging.

Introduction
Hyperspectral imaging of tissue could be used as a diagnostic tool for the detection of many diseases (Wang *et al.*, 2012; Ellis *et al.*, 2013; Aubertin *et al.*, 2017). However, many of these applications require imaging tissue samples; when producing such images, a need has been identified for techniques which are robust to interference from water, objective, non-destructive, and free from the need for tagging (Kast *et al.*, 2014). Raman imaging meets each of the stated needs, however it presents a new challenge. It can be highly time consuming, large images take several days to acquire. There is potential methods for reducing this time requirement. The instrument being used in this study, a Renishaw inVia Confocal Raman Microscope, operates by point mapping, acquiring a spectrum from a single point and then moving on to the next, or streamline imaging, using an elongated laser profile and passing it over the sample in a continuous movement to expose each 'pixel' of the final image for a pre-set time. Streamline imaging offers much faster acquisition of the final image at the cost of increased spectral noise. Point mapping, conversely offers clear spectra with much lower noise, but is affected by the afore mentioned time requirements.
One standard tissue preservation technique is fixation with formalin followed by imbedding in paraffin, this is convenient and long-lasting, making it ideal for research as it offers an unrestricted time frame for use of samples. However, spectral interference caused by the paraffin, can hide signals of interest from the tissue. Many overlapping bands have been noted between tissue and paraffin and various analytical methods have been attempted to remove the paraffin spectrum, with varying degrees of success (Patel and Martin, 2010; Gaifulina *et al.*, 2016; Meksiarun *et al.*, 2017). Another approach is to remove the paraffin by immersion in subsequent baths of xylene and ethanol, followed by rehydration in water to preserve the tissue architecture. This method physically removes the paraffin, and thus any spectral interference it caused. There is no standard method for the deparaffinisation-rehydration process, with different researchers using their own procedures or leaving them unstated (Nemolato *et al.*, 2008; Patel and Martin, 2010; Tollefson *et al.*, 2010). It is therefore necessary to develop a suitable method for future research to be carried out on deparaffinated samples.
The objective of this study was to determine the suitability of a method for the removal of paraffin from sections of tissue, and to compare the effectiveness of point mapping and streamline imaging in the acquisition of spectral information from the same tissue sections.

Materials and Methods

Section cutting:
A paraffin embedded prostate sample was provided by the Prostate Cancer Research Consortium (PCRC). Initially six 4μm thick sections were cut. Four sections were affixed to glass slides and two

to aluminium slides. Following initial analysis, a further six sections were cut, two in each 8µm, 10µm, and 16µm thicknesses. Each new sections was affixed to a glass slide.

Staining:
One of the 4µm sections on glass that had been deparaffinated was used for Haematoxylin & Eosin (H&E) staining, to provide a ground truth after analysis and demarcation by a pathologist.

Deparaffination:
Of the initial 6 sections, three on glass slides and one on aluminium were deparaffinated. This was done by immersing the slides for three minutes in subsequent baths of solvents in the following order: Xylene, xylene, xylene, EtOH 100%, EtOH 100%, EtOH 90%, EtOH 80%, H_2O.
One section of each thickness was deparaffinated using the above stated method, however due to residual paraffin being detected during analysis the second 10µm section was deparaffinated using a second method. The slide was first baked at 60^{o}C for one hour, the above procedure was then repeated on the baked slide with the immersion time doubled to six minutes.

Point spectroscopy:
Point spectra were acquired from each region of the background in order to correct and compare in the analysis stage of the experiment.
Point spectra were acquired from various regions on each of the unstained sections mentioned above.

Point mapping:
It was intended to create a point mapped image from a small area of tissue on each of the 4µm thick sections, however such images proved to be unattainable due to difficulties focusing on the surface of such thin sections.
Point mapped images of a small tissue area were created for each of the deparaffinated 8µm, and 16µm sections as well as both 10µm sections using 100% power from a 500mW, 532nm laser with 10 accumulations at an exposure time of 0.5s.

Streamline imaging:
The same area of both 10µm sections was imaged using the streamline setting on the instrument using 100% power from the same laser and an exposure time of 12s.

Pre-treatment:
The point mapped images showed some areas of detector saturation, these were removed using masks created from the principle components (PCs) found during principle component analysis (PCA).
Linear baseline correction was used in order to account for the skewed baseline caused by fluorescence in the samples.
The standard normal variate (SNV) of each spectrum was calculated and used to normalise the spectra of each image.
The first five PCs found from PCA of the masked and normalised images were used to reconstruct the images, allowing for much of the noise from the original spectra to be smoothed, producing clearer and more readable spectra.

Results and Discussion
The resulting images were analysed using in house functions for Matlab 2017b as well as the included Machine Learning and Signal Processing Toolboxes.
Analysis of the images included:

1. Unfolding the image data into two dimensional matrices, allowing pre-treatments to be applied to the data.
2. Overlaying paraffin spectra on the image spectra to check for residual paraffin.
3. Visual comparison of the spectra and images produced from point mapping and streamline images.
4. Rendering of scores produced by PCA of the final images.

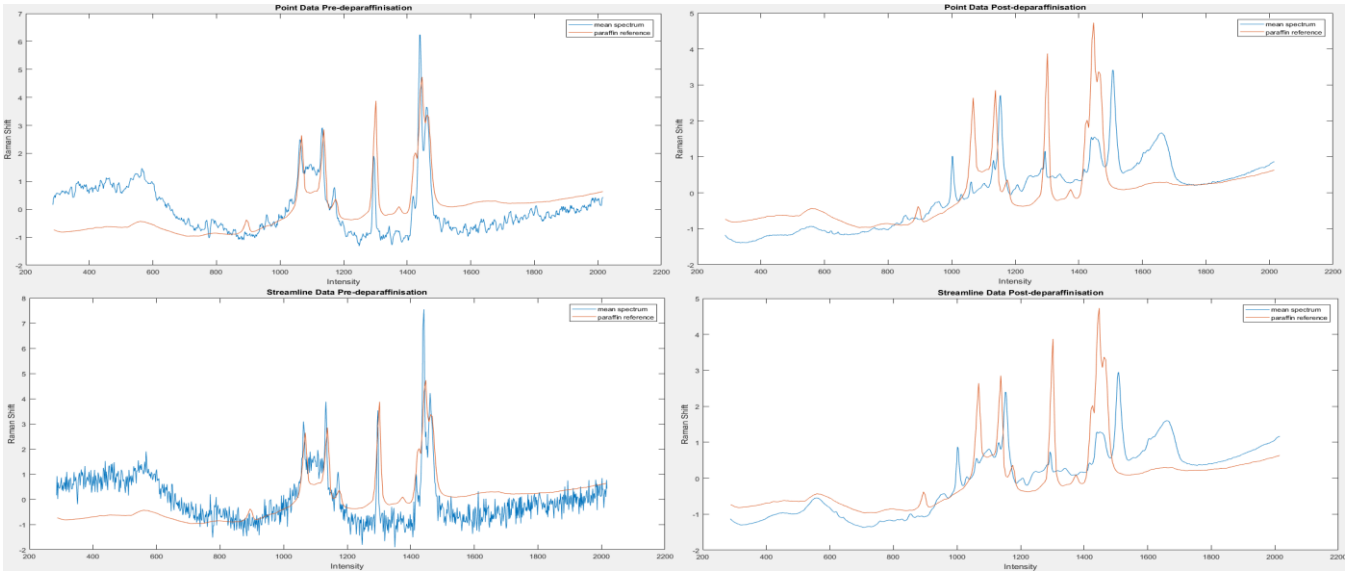

Figure 1: Mean spectra from point mapping data (top) and streamline data (bottom) before deparaffinisation (left) and after deparaffinisation (right), with a paraffin reference spectrum overlayed on each.

Strong interference from the paraffin was masking any information from the tissue before deparaffinisation. After deparaffinisation was conducted, some residual effect was still seen taking place. Paraffin peaks were still present at 1068nm, 1138nm, 1302nm, and a broad peak at 1416-1483nm. More intensive deparaffinisation techniques may remove residual paraffin (Nemolato *et al.*, 2008).

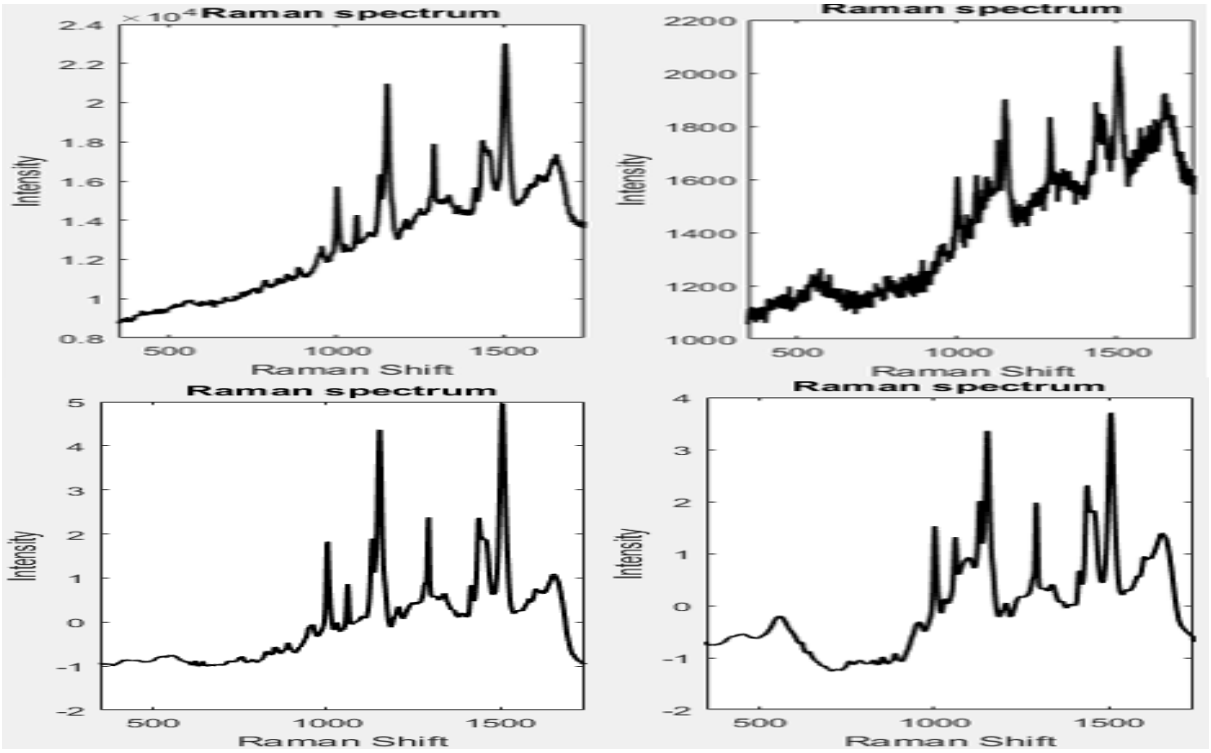

Figure 2: Spectra from the same location within the point (left) and streamline (right) images, before (top) and after (bottom) pretreatment.

The main advantage of the point mapping over streamline imaging was the clarity of the spectra it produced. The above figure (**Figure 2**) shows a distinct difference in clarity before pre-treatments. After the application of pre-treatments, the clarity of the two spectra is comparable, neither being significantly better than the other.

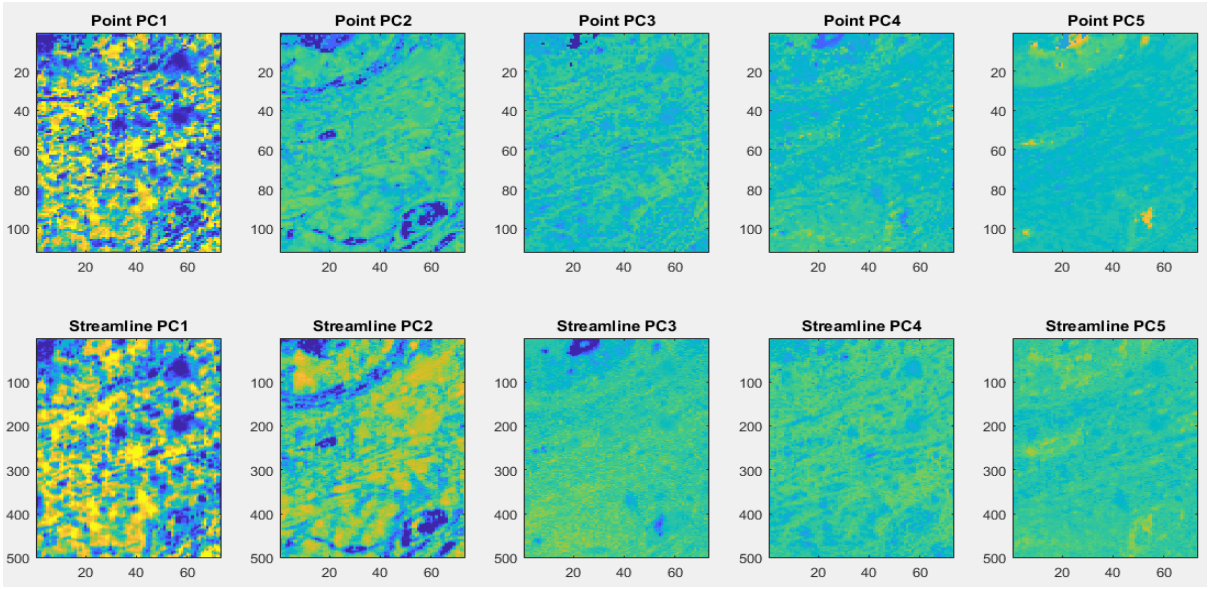

Figure 3: The first five principle components found in the treated point (top) and streamline (bottom) images.

PCA of the treated images showed similar results for both imaging technique, with some variation in intensity of the component signal in PC2 and PC5.

Conclusions

These preliminary results show promise for the use of streamline imaging as the primary image acquisition technique for Raman hyperspectral imaging of tissue when using this instrument. Examination of the results of imaging the tissue pre- and post-depariffinisation shows a clear need for the removal of paraffin before the commencement of image acquisition.

Acknowledgements

The authors would like to thank the Health Research Board (HRB) who funded this research.

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APPLICATION OF UV-VIS SPECTROSCOPY FOR ADULTERATION DETECTION IN GIN

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Abstract

In this study UV-Vis spectroscopy was utilized to detect gin adulterations in the spectral range between 200 and 500 nm in absorbance mode. Three different gin brands were used for this study. Gin samples were diluted with three common adulterants: ethanol, water, and a cheaper brand. Different gin adulteration levels were considered for the experimental set-ups, which consisted of a total of 151 samples. The spectra collected from the samples were pre-treated utilising Standard Normal Variate (SNV) and Savitzky–Golay smoothing and then analysed using Principal Component Analysis (PCA) and Partial Least Squares Regression (PLSR). After performing multivariate analysis, it was possible to obtain good models of prediction for water (square R of validation: 0.975; RMSE of validation: 2.17) and ethanol (square R of validation: 0.91; RMSE of validation: 4.05) adulteration, and an effective classification of the brands using PCA. Although UV-Vis spectroscopy produced noise in the spectra of the samples, pre-treatments reduced this problem and improved the multivariate analysis of the data.

Introduction

The adulteration of alcoholic beverages may be used to increase the alcoholic strength of a spirit, but sometimes it is combined dilution in order to maximize the profit of the counterfeiter. This fraudulent behaviour may have serious consequences for the consumers buying counterfeit spirits. Food and legal organization are engaged in a continuous fight against counterfeiters to protect both the rights of the customers and the authenticity of the brands at risk. It is necessary to develop rapid and robust analytic tools that can accurately assess the authenticity and the quality of beverage products. UV-Vis spectroscopy is a fast, non-invasive and non-destructive technology which can be effectively used for this purpose.

Spectroscopic sensors provide characteristic emission and absorption spectra, which are valuable information on individual substances and the composition of complex mixtures. Electronic transitions for example, are immensely energetic due to absorbance in the UV-Vis range. Organic molecules for example, are strongly excited in the UV and visible regions of the spectrum, involving multiple bonds such as: C=C, C=O, and C=N (Herold et al., 2009). Multivariate analysis is required to analyse UV spectral data.

The objective of this study is to investigate UV-Vis spectroscopy in combination with multivariate analysis to detect adulteration of Gin.

Materials and Methods

Four different brands of gin were obtained from licensed alcohol shops. A UV-3100PC Spectrophotometer (VWR International Limited, China) in absorbance mode, was used to collect spectra of gin samples in a wavelength range from 200 to 500 nm (range characterized by an absorption of poly-unsaturated and aromatic compounds Herold et al., 2009).

Three experimental studies were used in this study and a total of 151 samples were prepared. The first study aimed to analyse dilution of 3 brands of gin (Bombay, Mòr, Thin) with distilled water (adulterant/gin in volume: 0, 1, 2, 5, 10, 20, and 40%). The second study analysed dilution of 3 brands of gin with pure ethanol (adulterant/gin in volume: 0, 1, 2, 5, 10, 20, and 40%). The third study classified the dilution of gin with another lower cost brand (Hampstead). The experiments were repeated three times with different samples, randomizing

the dilutions order (to avoid ambience interferences). Once the spectra were obtained, UnScrambler v9.7 (CAMO Process, Oslo, Norway) was used to pre-treat the data and carry out PCA and PLSR.

Results

The first step of the multivariate analysis classified the gins' brands. Spectra of not-diluted gin samples were used for this purpose. Since a clear classification is hardly achievable using pure spectra, PCA was applied to the pre-treated data (Fig. 1a). From the PCA it is possible to identify four different clusters and differentiate the four brands using only the PC1 and PC2 (Fig. 1b).

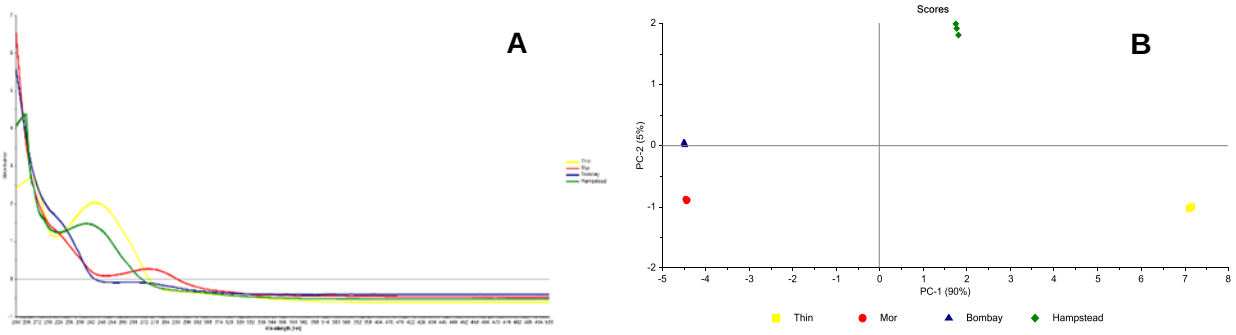

Figure 1: Spectra (pre-treated) of the four pure gin brands used for the study (A) and PCA of the same data (B).

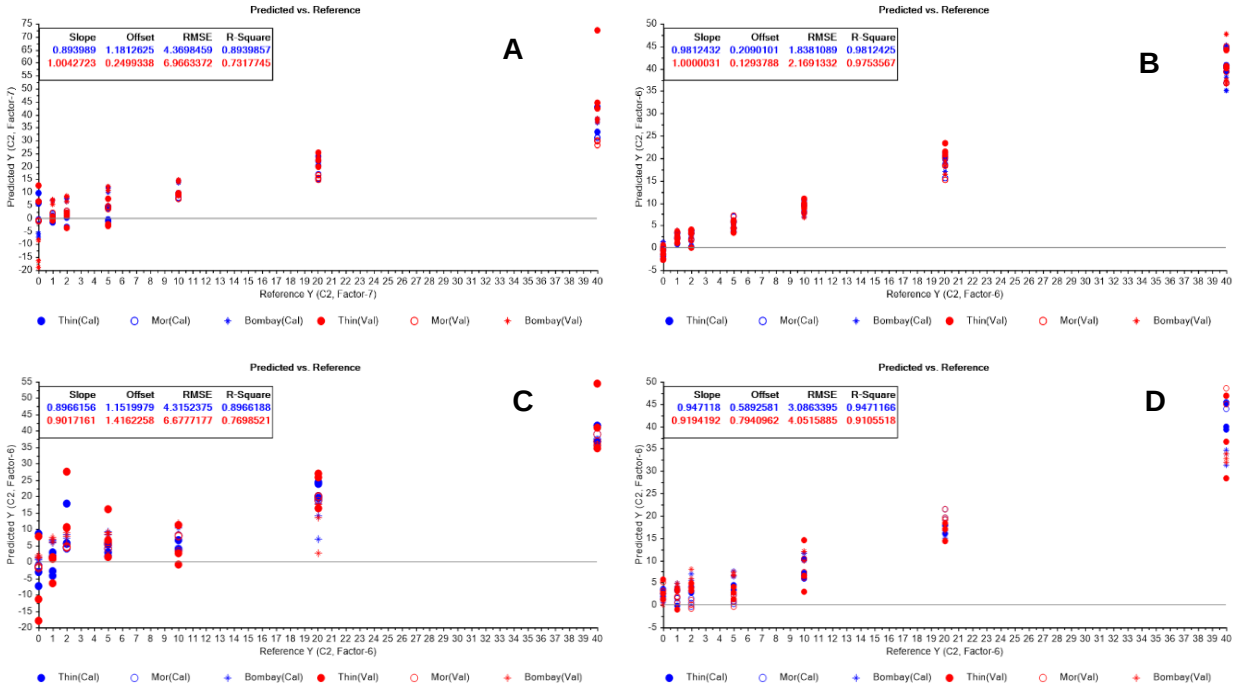

Figure 2: Models created applying PLSR to the spectra of three brands diluted with different quantities of distilled water (A without pre-treatments; B with pre-treatments) and pure ethanol (C without pre-treatments; D with SNV).

The second part of the study aimed to build models with PLSR. The models in Fig. 2A, B, C, and D were created using for every single dilution in gin, two repetitions for the cross validation and one for the validation.

Fig. 2A, B show the model obtained from the spectra of three brands of gin diluted with distilled water. The two models prove how the pre-treatments improve the final prediction, reducing RMSE (validation from 6.96 to 2.17) and increasing square R (validation from 0.73 to 0.97).

Fig2C, D show the model obtained from the spectra of three brands of gin diluted with pure ethanol. In this case, Savitzky–Golay smoothing reduces the effectiveness of the prediction model, making SNV the only pre-treatment used for the optimization of the PLSR. PLSR applied to pre-treated data (only SNV), brings to improvement of RMSE (validation from 6.7 to 4.05) and square R (validation from 0.77 to 0.91) values.

The last part of the study analyses of the dilutions of Mòr (the most expensive of the four brands) with Hampstead (the cheapest of the four). PCA was firstly applied to the data without pre-treatments in Fig. 3C. However, the classification of the dilutions of Mòr with Hampstead is possible only with pre-treated data. The dilution of Hamptead in Mòr seems to create a new product, moving away from the original spirit.

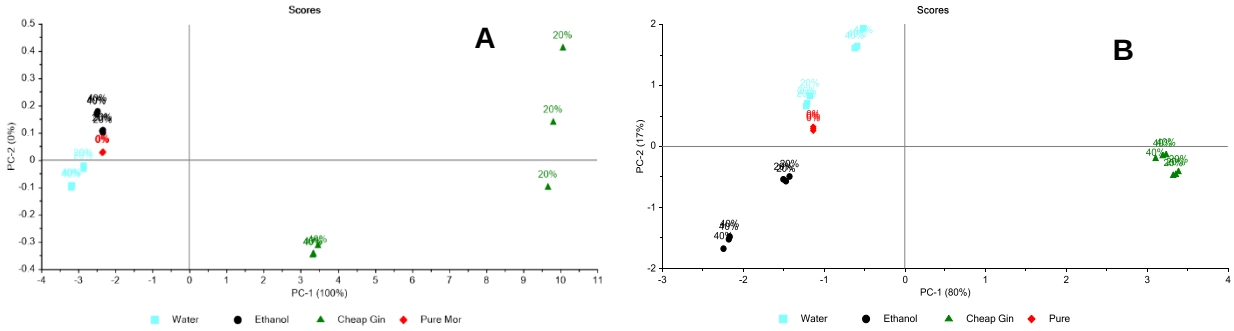

Figure 3. PCA applied to the spectra of Mòr diluted with different quantities of Hampstead (adulterant), with (B) and without (A) pre-treatments.

Conclusion

The results of this study demonstrate that UV-Vis can be used to predict adulteration in gin samples. However, it is important to emphasize the large impact of pre-treatments in the multivariate analysis. Pure UV-Vis spectra presented phenomena of interference at the start and at the end of the spectral wavelengths rage utilized for the study (200-500 nm). SNV and Savitzky–Golay smoothing permitted to overcome those problems improving the data analysis. PCA was applied in each experimental design, allowing a clear classification per brand. PCA resulted to be effective for the classification of dilution of Mòr with Hampstead.

PLSR was used to create prediction model for dilution of gin with water and ethanol. This technique provided accurate predictions of the water dilutions in gin, achieving good values of square R of validation (0.975) and RMSE of validation (2.17). Ethanol dilutions in gin, offered a less accurate prediction, achieving lower values of square R of validation (0.91) and RMSE of validation (4.05). In conclusion, differently from water, ethanol adulteration resulted to be harder to predict due to its high volatility.

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Jiani Luo, BE, M.EngSc., M.Sc.

Project Title: Applying PAT tools to monitor milk coagulation in cheese manufacture.

Project Leader: Dr. C. Esquerre, Prof. Colm O'Donnell

Abstract

Milk coagulation is an important step in cheese making processing which can affect final product's nutritional and sensory quality (Fox, 2004). It is necessary to explore an effective tool for monitoring milk coagulation in cheese processing. The objective of this study was to monitor milk coagulation in real-time by NIR, fluorescence spectroscopy and rheometer. Rheological analytical methods can determine physical cheese gel characteristics, e.g. storage modulus G' (Lucey *et al*., 2003), that cutting time is directly dependent on. NIR, fluorescence data can be used for predicting cutting time in cheese producing. For this purpose, data was collected in a cheese plant. The milk samples were obtained from multiple cheese vats after rennet addition. The data was analyzed by chemometric analysis (multivariate data analysis), PCA and PLS models were established and tested on 152 cheese batches. The data analysis procedure was followed by selecting samples reach 20 Pa based on rheometer reference data and find the time at the sample reach to the 20 Pa as the target cutting time. Then, three data pre-treatment methods were applied: scale, SNV and Savitzky-Golay filter. After that, PCA and PLS model were built by temperature, NIR and fluorescence pretreated data to predict cutting time. Finally, the models were validating 10 times by randomly selected samples not used for building models. The best result is the PLS model built by Scaling and Savitsky-Golay pretreated data, it can predict the cutting time with root mean square error (1.8 min and standard deviation = 0.18 min). It is big improvement by applying this PAT tool due to the variation of cutting time at 20 Pa could be 10 min or more in the industry. Therefore, this study can demonstrate a PAT tool for real-time modelling of milk coagulation in the real industry environment which could potentially applied for better control and optimization of cutting point in cheese production.

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EFFECT OF SPECTRA STANDARD PRETREATMENTS ON NEAR INFRARED, RAMAN AND FOURIER TRANSFORM HYPERSPECTRAL IMAGING OF WHOLE MILK ON ALUMINIUM

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Abstract

Milk is a complex emulsion of fat and water, proteins (caseins and whey protein), vitamins, minerals and lactose are dissolved within. Milk has an important role in the human diet, it is consumed in liquid form or within a dairy product. In this study the effect of Multiplicative Scatter Correction (MSC) and Standard Normal Variate (SNV) on Near Infrared (NIR), Fourier Transform Infrared (FTIR) and Raman hyperspectral imaging of whole milk on aluminium was investigated. This material was chosen as a candidate surface due to its widespread use in food production.

Introduction

Milk has an important role in the human diet, it is consumed in liquid form or as a dairy product. It is therefore necessary to investigate milk and dairy products in terms of hygiene and safety and also in terms of composition and nutrients. Milk is a complex emulsion of fat and water, proteins (caseins and whey protein), vitamins, minerals and lactose are dissolved within (Mckenzle, 1967). Its complex nature makes it difficult to completely characterise with a single technique for all components quickly. In chromatography it is difficult to determinate common parameters to separate all milk components (Pellegrino and Tirelli, 2000; Bonfatti *et al.*, 2008). Spectroscopy is a technique widely used to characterise their composition. Fat micelles affect light scattering in NIR (Cattaneo *et al.*, 2009). A clear signal for fat and protein is evident in Raman (Mazurek *et al.*, 2015) and FTIR spectroscopy provides lactose information (Iñón *et al.* ,2004).

In this study, a combination of Near Infrared (NIR), Fourier Transform Infrared (FTIR) and Raman hyperspectral imaging were used. Hyperspectral imaging helps to combine chemical information with spatial information. From previous studies, it was possible to predict the type of information that each technique can provide. Aluminium was chosen as a candidate surface due to its widespread use in food production (Jullien *et al.*, 2003). Spectra of dried samples of whole milk on aluminium were collected with the different techniques. The use of an aluminium surface introduces another parameter to consider in the experiment: roughness. It demonstrates the important of application of hyperspectral imaging against point spectroscopy. In addition, the spectroscopic information collected is not only affected by the chemical signal of the milk composition, but it is also possible to observe surface-related signals, evident in baseline and multiplicative effects. The study and interpretation of these effects can be used to investigate the interaction between surfaces and dairy residues. In addition, the combination of the spectral information with spatial information can improve data interpretation in terms of characterising spatial variability in the selected surfaces.

Multiplicative Scatter Correction (MSC) and Standard Normal Variate (SNV) are both row-wise pretreatments that rescale spectra. They are widely used in spectroscopic data analysis, especially in NIR spectroscopy. Both, MSC and SNV are presented as methods to eliminate the noise and the scatter between spectra. They eliminate the multiplicative and additive effects due the light scattering. They differ in that MSC works uses a spectrum as a target and rescales all other spectra based on it. SNV utilises the mean and standard deviation of each spectrum. Practically, applying these pretreatments to HSI spectra, results in different rescaling of the spectra. When the mean spectrum of the image is used as a target in MSC it can be said that each pixel contributes to all others. SNV rescales each spectrum/pixel independently. A theoretical study about the link between the two method was published in 1995 (Dhanoa et al., 1993).

In this paper, the effect of MSC and SNV pretreatments on whole milk spectra were studied.
Materials and Methods

Materials
The chosen surface was aluminium slide (37mm × 25mm × 1mm), it was purchased from Rice Metals Ltd. (Cornwall, United Kingdom).
Avonmore whole milk was used for this analysis. It was purchased from local store.
To clean the surface a solution of ethanol/acetone (1:1 v/v) was used. Ethanol 99%, Absolute, Extra Pure, SLR was purchased from Fisher Scientific Ltd. (Dublin, Ireland) (CAS Number : 64-17-5) and Acetone (HPLC) obtained from Fisher Scientific Ltd. (Dublin, Ireland) (CAS Number: 67-64-1).
Deionised (DI) water, to clean the surfaces after the solution ethanol/acetone, was sourced from a Thermo Scientific™ Barnstead™ Smart2Pure™ water purification system producing Type I ASTM water, with a resistance of 18.2 MΩcm at 24.7 °C.
Grace Bio-Labs Press-To-Seal silicone isolators are used to applied the milk on the surface. They were adhesive on one side. They were round with 13mm of diameter and 2.5mm depth. they were purchased from Sigma-Aldrich (Wicklow, Ireland).

Method
Sample preparation
Each surface was cleaned with a solution of ethanol/acetone (1:1 v/v) for 5 minutes to avoid any trace of glue from the protective layer and rinsed three times with deionised water. The isolator was applied on the top and filled with 3 mL of whole milk.

Hyperspectral imaging
Recent technological developments have also influenced spectroscopic analysis. Hyperspectral imaging (HSI) derives from the combination of classic spectroscopy and spectral imaging.
Hyperspectral imaging produces digital data. However, in this case each pixel has a third dimension. This third dimension is the spectrum collected by the instrument at a specific point, stacking images of the same area recorded at different wavelengths (Gowen *et al.*, 2007). There are different ways to work with HSI:
"Whiskbroom" or "point mapping",
"Pushbroom" or "line scanning",
"Staredown" or "staring face". (Gowen *et al.*, 2015).
In this study, the HSI techniques used were:

- Raman wavenumber range was 190-3900 cm^{-1} using an edge laser for excitation at 785 nm. The laser was, set to 5% power (power measured at source was 306 mW) with a 5 s acquisition time for each spectrum. Images were obtained using a 10x 0.25 NA objective lens. Average spectral resolution: 1.5494 cm^{-1}.
- FTIR spectra were acquired over the range 475-7500 cm^{-1}. Each spectrum was a mean of 16 acquisitions with a total acquisition time 5s per spectrum in reflectance mode, aperture size 150 x 150 µm and step size of 150 µm. Average spectral resolution: 1.928 cm^{-1}.
- NIR (DV Optics, Padua, Italy) images were collected in reflectance every 7 nm over the range 880-1720 nm. The speed was 20 $mm.s^{-1}$ using a pushbroom system.

Data analysis
Multiplicative Scatter Correction (MSC). It is a spectra correction base on an ideal spectra.

$$x_i = b_0 + b_1 x_{ref} + \varepsilon$$

$$x_{imsc} = \frac{x_1 - b_1}{b_1}$$

x_i raw spectra
x_{ref} target spectrum
x_{i_msc} corrected spectra
b_0 coefficient offs
b_1 coefficient multiplicative effect.
ε error

There are different ways to apply this pretreatment based on the concept of a target spectrum. It is possible to identify part of the real spectrum as an ideal spectrum, where no peaks or chemical signals are present. This method may be affected by low ratio signal to noise. In this study, the mean for each modality was calculated from the whole spectrum and applied as an ideal spectrum.
Standard Normal Variate (SNV). A row-wise operation.

$$x_{ij} = \frac{x_{ij} - \underline{x}_i}{\sigma_i}$$

σ_i is standard deviation of i row

$\underline{x}_i$ is the mean of i row.

SNV is defined as "a normal variate with mean $\mu = 0$ and standard deviation $\sigma = 1$". As mentioned before it processes every spectrum individually, eliminating the additive and multiplicative effects related to light scattering (Barnes et al., 1989).

Results and Discussion

Figure 1 (a-c) shows the spectra of a sample of dried whole milk, prepared as described in the "Material and Method" section, with FTIR in reflectance mode, Raman, NIR spectroscopy. The spectra with SNV and MSC applied are presented in Figure 1 (d-f) and Figure 1 (e-i) respectively. In addition, the mean spectra of aluminium are reported for each spectroscopic technique Figure 1 (j-k).
It is possible to observe the scattering in the spectra was eliminated with both SNV and MSC pretreatments. The eliminated scattering is due to irregularity on the scanned surface. This effect is more evident with HSI, than classic point scan spectroscopy. By collecting the data of an entire surface, it is possible to measure the chemical signal of the surfaces, as with the classic point spectroscopy but also measure the physical effect of properties of the material such as, roughness.
Independently rescaling the spectra, i.e. using SNV, seems not to underline any significant difference than when considering the relation between pixels (MSC). Examining the NIR spectra carefully, Figure 1 (f) and (i), it is possible to recognise some subtle differences around 1200 nm. As large differences are not presented between these pretreatments, it is possible to hypothesise that the investigated sample was homogeneous.

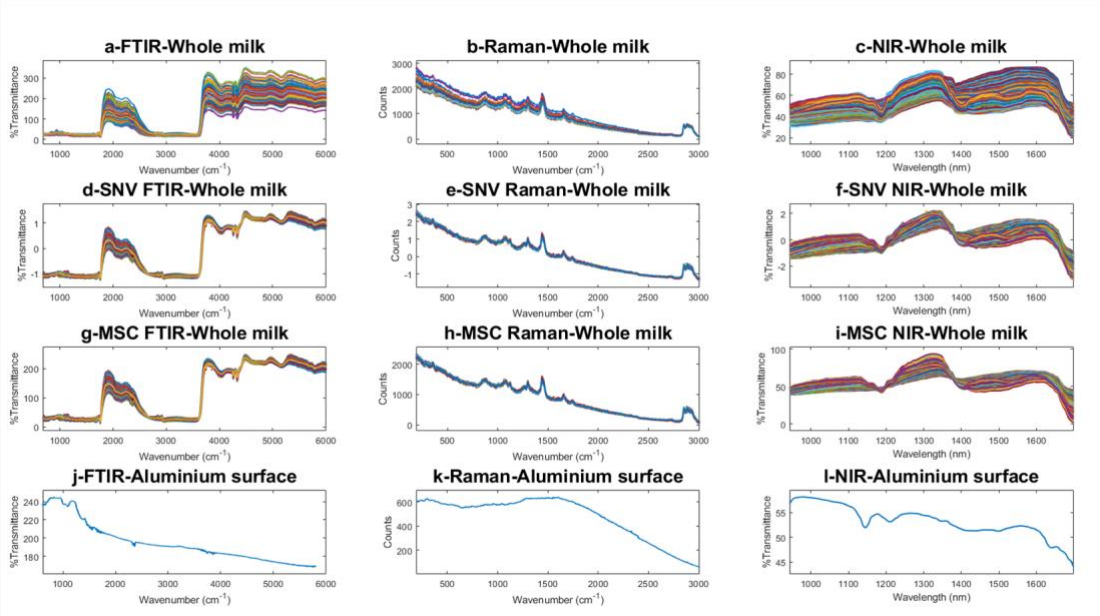

Figure 1. Plot of whole milk spectra on aluminium surfaces, (a-c) raw data of FTIR, Raman and NIR, respectively; (d-f) SNV applied to FTIR, Raman and NIR, respectively; (g-i) MSC applied to FTIR, Raman and NIR respectively. (g-i) Aluminium surface raw data of FTIR, Raman and NIR, respectively.

Comparing the pretreated spectra and the raw spectra with the spectrum of pure aluminium for each technique, it is possible to see a clear influence of the surface material on the milk spectra. In FTIR spectra the same pattern as aluminium is present around 1000 cm^{-1}. In addition, the Raman baseline seems to be affected by the surfaces. In the case of NIR, this influence is present in the baseline trend but also in the peaks around 1100-1200 nm

Conclusions

The comparison between the application of MSC and SNV pretreatments on the HSI data of whole milk on aluminium surfaces does not underline any significant difference between these two methods. In this case it is possible to hypothesise a homogeneity of the sample and its interaction with the surface. On the other hand, observing pure aluminium mean spectra, it is evident that this affects each of the techniques. This consideration opens up future investigation about the interaction between aluminium and milk the development of improved chemometrics pretreatments.

Acknowledgements

Funding for this research was provided by Science Foundation Ireland (SFI) under the investigators programme Proposal ID 15/IA/2984—HyperMicroMacro.

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PRELIMINARY STUDIES ON NIR HYPERSPECTRAL IMAGING IN VISUALIZING MOISTURE DISTRIBUTION OF MUSHROOM SLICES DURING MICROWAVE-VACUUM DRYING

Xiao-Hui Lin, Da-Wen Sun*, Jun-Li Xu
Food Refrigeration and Computerized Food Technology (FRCFT), UCD School of Biosystems and Food Engineering, University College Dublin, Belfield, Dublin 4, Ireland.

Abstract

The moisture content (MC) of the mushroom slices being processed during microwave-vacuum drying (MVD) is crucial to evaluate the qualities of final drying mushroom slices. Near-infrared (NIR) hyperspectral imaging in combination with multivariate chemometric analysis were employed for moisture prediction. A model based on the full range wavelengths was developed using partial least squares regression (PLSR) and applying spectral pre-treatment of a SNV to the mushroom slice hyperspectral images, resulted in the best model performance. An optimized PLSR model, achieving a high prediction accuracy with R_{cv}^2 = 0.967 and RMSECV = 5.22%. The result shows that the NIR hyperspectral imaging technique is a promising tool for non-destructively and rapidly measuring and visualizing the moisture content of mushroom slices during MVD.

Introduction

Mushrooms are widely planted and consumed in the world. Mushrooms are popular for their favourable characteristics, including a low calorific value, high vitamin B and mineral content (Walde *et al.*, 2006). Mushrooms are always served as fresh, but are very perishable. Dried mushrooms have a long shelf-life and they take much less storage space than fresh mushrooms. Dried mushrooms are widely used in a variety of dishes such as instant soups, rice dishes, snacks, pizzas, and sauces (Giri and Prasad, 2013).

The microwave-vacuum drying combines the advantages of microwave heating and vacuum drying, and is a promising drying technique of preserving food. MVD had been reported to shorten the drying time, improve the rehydration ratio, reduce energy consumption, and reduce the nutrient lost (Jiang *et al.*, 2016). However, non-uniform heating during microwave processing would cause microbial safety concerns, and overheating (Vadivambal and Jayas, 2010). This non-uniform characteristic could be evaluated by the moisture distribution of the product.

Hyperspectral imaging technique which combines spectroscopy and imaging techniques has been applied to the research of the non-destructive and fast detection in agriculture products. The detection of moisture content of the food has proved to be feasible. Taghizadeh *et al*. (2009) had reported that hyperspectral imaging was able to predict the mushroom moisture content. Pu and Sun (Pu and Sun, 2015) demonstrated the potential use of hyperspectral imaging as a tool to measure and visualize the MC during MVD process of mango slices.

The objective of this study was to determine the moisture distribution of mushroom slices during microwave-vacuum drying using hyperspectral imaging technique.

Materials and Methods

Sample preparation
Mushrooms (*Agaricus bisporous*) with a diameter of 3-5 cm were purchased from the local supermarket and kept in cold storage at 4-5 °C. The mushrooms were sliced into pieces of 5 mm thickness by a stainless-steel slicer. The slices from middle portions with characteristic mushroom shape were used for microwave vacuum drying experiments.

Drying procedure
The MVD system was described as the previous study (Pu and Sun, 2015). Briefly, the microwave power of 250 W and the vacuum pressure of 15 ± 2 mbar were set for the MVD. A circulation of two-minute heating-on and one-minute heating-off of microwave oven was carried out to avoid overheating. Eight groups of drying experiments (with the different microwave heating time of 0, 6, 12, 18, 24, 30, 39, and 48 min, respectively) were carried out. In each group, twenty slices were used and about 25 g of mushroom slices were taken for each MVD experiment, resulting in 160 samples. Moisture contents of the samples were measured by the oven method: mushroom slices were dried at 105 °C until the constant weight was obtained. The moisture content were evaluated by mass difference and showed as a wet base percentage.

Hyperspectral images acquisition
The NIR hyperspectral imaging system used is similar to that used by He *et al*. (2013).

Data pre-processing
All pixels in the image corresponding to the mushroom slice were separated from the background and dead pixels, and considered as the region of interest. The pre-processing of standard normal variate (SNV) was used to eliminate scattering effect of the sample. Corrected spectra were obtained by mean centring and scaling by its standard deviation.

PLSR modelling and visualization
The quantitative models between the MC and the spectral data of the mushroom slices based on diverse spectral pre-processing methods covering the raw spectra and those modified by SNV were established by PLSR. PLSR is a widely used method for constructing regression models when the measured variables are highly collinear. Samples were divided into a calibration set (70%) and a prediction set (30%), and cross-validation was performed in the calibration set. The root mean square error (RMSE) and coefficient of determination (R^2) were used to determine the accuracy of each calibration model. The model with lowest RMSE and highest R^2 was the optimised PLSR model. In current study, the optimised PLSR model was applied to each pixel of the spectral cube to build the moisture distribution map of the mushroom slice.

Results and Discussion

Drying kinetics and spectral characteristics of the mushroom slices
The drying curves for thin layer drying of mushroom slices under MVD conditions are shown in figure 1 (a). The MC of the mushroom slices decreased from around 90% to around 10% within 48 min of MVD. At 30 min and 39 min of MVD, the MC of the mushroom slices showed significant difference at the same heating time. These were attributed to the inherent non-uniform temperature distribution, which was induced by uneven spatial distribution of the electromagnetic field inside the drying cavity (Wang *et al.*, 2013). Figure 1 (b) shows the relative reflectance of mushroom slices with different moisture contents (3.75%, 71.81%, and 93.87%). Obviously, the mushroom slices with higher MC had relatively lower reflectance intensities.

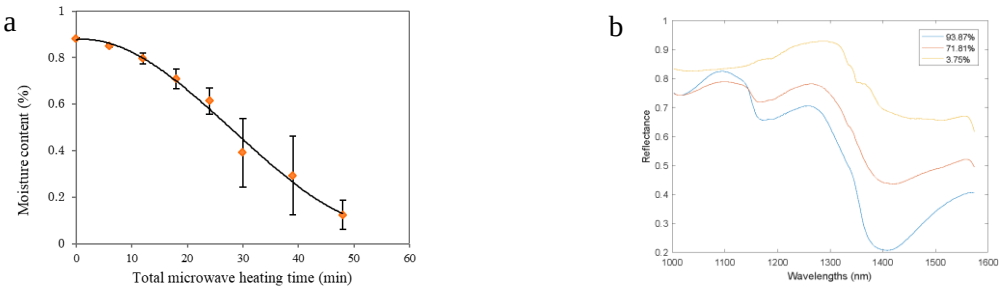

Figure 1. (a) Drying curves of microwave-vacuum dried mushroom slice and (b) spectral profiles of mushroom slices in the spectral range of 1002-1575nm.

Pre-processing and PLSR models

According to the Figure 2, the SNV could significantly eliminate the scattering effect. In addition, table 1 shows that the PLSR model based on SNV method had a relatively good performance, with lower RMSE and higher R^2. Thus, the PLSR model based on SNV method was the optimised PLSR model, which would be further employed to predict MC in mushroom slices during MVD.

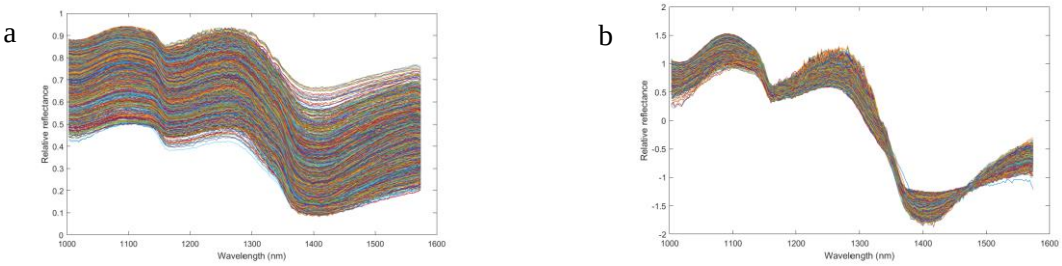

Figure 2. Spectral pre-processing for raw NIR spectra of mushroom slices. (a) Original spectra and (b) pre-processed spectra with SNV.

Table 1. Moisture prediction performance of PLSR models with and without SNV pre-treatment

Pre-processing	LVs	RMSEC (%)	RMSECV (%)	RMSEP (%)	R_C^2	R_{CV}^2	R_P^2
None	4	9.419	10.104	9.958	0.899	0.883	0.889
SNV	4	4.957	5.220	4.073	0.970	0.967	0.950

RMSEC, RMSECV, and RMSEP were calculated from the calibration set, cross-validation set and prediction set, respectively. Similarly, R_c^2, R_{cv}^2, and R_p^2 were calculated from the above sample sets.

Visualization of moisture content

Figure 3 displays the distribution map of MC in eight mushroom slices during MVD. The mushroom slice with MC of 93.87% was the fresh one without any pre-treatment and showed the uniform distribution of MC. During the MVD, the colour of the cap tended to the red side of the linear colour bar, while the colour of the stipe tended to the blue side, which indicated that the moisture was likely to run off faster from the cap than the stipe.

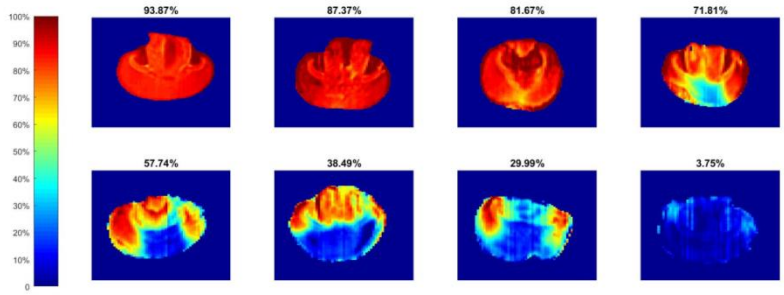

Figure 3. Moisture distribution maps of mushroom slices generated by using the optimal PLSR model.

Conclusions

NIR hyperspectral imaging technique combined with data pre-processing and modelling made it possible to visualize the moisture distribution in mushroom slices during microwave vacuum drying. The PLSR model based on SNV method had a good performance in the predication of MC. The MC distribution maps of the mushroom slices indicated that the evaporation rate of moisture in the cap of the mushroom slice was higher than the stipe during MVD process.

Acknowledgements

This research was funded under the UCD–CSC Scholarship Scheme between University College Dublin (UCD, Ireland) and Chinese Scholarship Council (CSC, China).

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Kexin Zhang, PhD

Project Title: The effect of plasma treatments on rheological properties on tapioca starch

Project Leader: Dr. Brijesh Tiwari and Prof. Da-Wen Sun

Abstract

Starch is the most abundant reserve carbohydrate in plants and the most common used polysaccharide in human diet. What's more, it also has many industrial applications such as thickener, colloidal stabilizer, gelling agents, bulking agent, water retention agent and adhesive. There is a high potential explore its chemical modifications during food processing. The objective of my research is to investigate the effect of different gases induced plasma treatments on rheological properties of tapioca starch. In this research, 18 samples of native tapioca starch (2 control samples, 16 treated samples) were used. The samples in treatment groups were treated in a bell-jar DBD plasma system under different gas agents (composed air, CO2, Argon and helium, respectively) by 20 or 30 min. Then the changes in starch rheological properties were estimated by Rapid Visco Analysis (RVA). During RVA test, controlled temperature (50-90 °C) and shear speed (0-960 rpm) were applied on the samples, showed in Table 1.

Table 1: RVA General Pasting Method

Time	Type	Value
00:00:00	temperature	50 °C
00:00:00	speed	960 rpm
00:00:10	speed	160 rpm
00:01:00	temperature	50 °C
00:04:42	temperature	95 °C
00:07:12	temperature	95 °C
00:11:00	temperature	50 °C

After analysis by *SPSS statistic*, significant differences between plasma treated tapioca starches and control samples were found on viscosity values of pleak1, trough1, and breakdown as well as peak time.

In a conclusion, different gases mediated plasma treatments have effects on tapioca starch rheological properties, in terms of peak viscosity, trough viscosity, breakdown viscosity and peak temperature. However, the mechanisms causing these changes still need to be further investigated.

Ronan Dorrepaal

Project Title: The development of chemical imaging and chemometric techniques to investigate fundamental biomaterial interactions with biological systems

Project Leader: Assoc. Prof. Aoife Gowen

Abstract

A biomaterial is traditionally defined as "any substance (other than a drug) or combination of substances, synthetic or natural in origin, which can be used for any period of time, as a whole or as a part of a system which treats, augments, or replaces any tissue, organ, or function of the body" (Galletti and Boretos 1983). Our research aims to characterise the *in vitro* and *ex vivo* degradation of biomaterials, and in particular, the heterogeneity of surface degradation. The research also seeks to examine the effect of biomaterial degradation on the fundamental interactions of biomaterials with biological systems. Hyperspectral chemical imaging systems were used to investigate material surface heterogeneity. Such systems collect spatially mapped spectra, allowing the generation of a chemical map of a material surface. The research employs the use of a range of hyperspectral chemical imaging modalities, including Raman scattering and mid-infrared, near-infrared and visible light. In addition, studies have been conducted using ATR-FTIR and darkfield imaging arrangements. The collected data were processed through the use of machine learning techniques with a focus on the development of new chemometric algorithms. Polycarbonate urethane (PCU) components of explanted spinal implants and magnesium oxychloride (MOC) cements with potential for use in the regeneration of bone were both studied. It was found that, though point spectroscopy has been used as a measure of the surface degradation of PCU spinal implants, surface degradation varies considerably at the local level. Therefore, the use of point spectroscopy may lead to an over or under estimation of the extent of material degradation. The study also found that even PCU materials with little to no oxidative treatment showed some surface heterogeneity. Future work will study the effects of the measured surface variation in terms of both mechanical performance and biocompatibility.

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Selected Recent Publications

Dorrepaal, R., Malegori, C., Gowen, A. (2016) 'Tutorial: Time series hyperspectral image analysis', *Journal of Near Infrared Spectroscopy*, 24(2), 89–108

Dorrepaal, R.M., Lawless, B.M., Burton, H.E., Espino, D.M., Shepherd, D.E.T., Gowen, A.A. (2018) 'Hyperspectral chemical imaging reveals spatially varied degradation of polycarbonate urethane (PCU) biomaterials', *Acta Biomaterialia*, in-press

Acknowledgements:

This study was supported by the European Commission under the 7th Framework Programme (Grant agreement nos.: 604935 and 335508).

Le WEN, BSc

Project Title: Ultrasound assisted extraction of bioactive compounds from coffee silver skin with study of extraction kinetics

Project Leader: Prof. Da-wen Sun and Dr. Brijesh K Tiwari

Abstract

Currently employed techniques for extraction of bioactives require long extraction times and have low extraction efficiencies. There is a need to develop novel extraction methods with improved extraction rates and yields. Ultrasound is a potential novel extraction technology which can be considered as clean, green and efficient alternative to conventional extraction technologies. This study investigated the ultrasound assisted extraction of bioactive compounds including phenolics and caffeine from coffee silver skin. In addition, it studied the effect of ultrasound pre-treatment on bioactive extraction kinetics. Ultrasound pre-treatment was carried out using 6 grams of coffee silver skin powder mixed with 300ml of solvent. Ultrasound pre-treatment was applied for 10 min at the ultrasound powder of 20% and 100%. Whereas, control samples were with no ultrasound pre-treatment employed. All the samples were transferred to an orbital operating at a constant speed of 210 rpm under the temperature of 50°C. Samples were withdrawn after 0.5, 1, 2, 3, 4, 5, 6 and 24 h, and then were analyzed for total phenolics. Peleg's kinetic model was fitted to the experimental data obtained for extraction of total phenolics. In the study, quantification was processed for caffeine content, 3-chlorigenic acid, 4-chlorogenic acid and 5-chlorogenic acid by ultra-high pressure liquid chromatography (UPLC). Antioxidant activity was tested including DPPH and FRAP. Final samples were characterized for polyphenols by LC-MS. The result showed that the yield of total phenolics and caffeine increased with increasing ultrasound amplitude level. Total phenolics content was significantly higher ($p < 0.05$) for 80% methanol extraction compared to water extraction for all treatments. After 24 h of shaking on an orbital shaker, the highest concentration of extracted phenolics using water as solvent was 6.30 ± 0.02 mg GAE/gdb at 100% ultrasound amplitude level. The lowest value obtained was 5.88 ± 0.09 mg GAE/gdb in the case of control. Similarly the concentration of extracted phenolics after 24 h of shaking using 80% methanol as solvent was 8.85 ± 0.09 mg GAE/gdb at 100% ultrasound amplitude level. The lowest value obtained was 8.49 ± 0.46 mg GAE/gdb in the case of control. A similar trend was observed for caffeine The profile of the bioactive extraction curves showed an initial high rate of extraction followed by a much reduced rate asymptotically approaching an equilibrium concentration. The extraction yield of bioactives was time-dependent and increased with extraction time, especially over first 2 h of shaking. The extraction rate of solutes increases, but the increment of the extraction rate reduces with time and remains constant. At the experimental conditions investigated in this study, the yield and the kinetics of solid–liquid extraction of coffee silver skin bioactives were shown to be strongly influenced by solvent type and ultrasound amplitude level. This study demonstrates that ultrasound can be employed to enhance the efficiency of bioactive extraction from coffee silver skin. The bioactive extraction kinetics presented provides valuable data for scaling-up and process design of extraction systems.

Sindhuraj Mukherjee

Project Title: Development of chemical imaging techniques to understand the water – polymer interface.

Project Leader: Assoc. Prof. Aoife A. Gowen

Co-Supervisor: Dr. Jose Angel Martínez-González

Abstract

The polymer-water interface is not fully understood and the data generated from studying this interface can give novel information on biocompatibility, biodegradation and biofouling. My objective is to explore the feasibility of chemical imaging(Mukherjee and Gowen 2015), particularly in the infrared range, and develop methods to characterize a range of surfaces and interfaces involved in biocompatibility and biodegradation. The hydrophobicity of polymeric surfaces is known is to be involved in these processes, and water contact angle (WCA) acts as a macroscopic indicator of hydrophobicity. However, WCA acquisition is challenging and time consuming. Reference characterization of polymeric surfaces was done using WCA evaluation and compared to chemical imaging data. Our findings indicated the suitability of using certain spectral regions in the infrared range to indicate hydrophobicity of polymeric surfaces(Mukherjee *et al.* 2017). This has been further expanded to a larger set of polymeric surfaces with a wide range of hydrophobicity to construct a multivariate model with which prediction in spatial variations of hydrophobicity was made possible (submitted for peer review). The next step involves carrying out biocompatibility and biodegradation experiments, which are currently underway.

This project is funded by the European Research Council Starting Grant programme (ERC-SG-335508).

Selected Recent Publications

Mukherjee, S., Gowen, A. (2015) 'A review of recent trends in polymer characterization using non-destructive vibrational spectroscopic modalities and chemical imaging', *Analytica Chimica Acta*, 895, 12–34.

Mukherjee, S., Martínez-González, J.A., Stallard, C.P., Dowling, D.P., Gowen, A.A. (2017) 'Can attenuated total internal reflection-Fourier transform infrared be used to understand the interaction between polymers and water? A hyperspectral imaging study', *Journal of Spectral Imaging*, 1, 1–13.

Wen-Hao Su, B.Eng, M.Agr., PhD

Project Title: Quality evaluation of tubers and cereal flours by using spectral imaging

Project Leader: Prof. Da-Wen Sun

Abstract

Staple foods including cereals and root/tuber crops dominate the daily diet of human by providing valuable protein, starch, oils, minerals and vitamins. Combining the techniques of spectroscopy and computer vision into one system, spectral imaging technique with proposed chemometrics (such as PLSR, MLR, and SVM) was introduced in this study for simultaneous detection of both spectral and spatial information of food products. In addition to the ability for classifying tubers into different quality grades and gaining rapid information about tuber chemical components (such as moisture, starch, and dry matter) and physical attributes (texture, water binding capacity (WBC), and specific gravity (SG), infrared (IR) imaging spectroscopy is able to determine impurities of specific flour with avoidance of extensive sample preparation. Overall, it is promising for IR imaging spectroscopy to be used for food quality determination.

Selected Recent Publications

Su, W.-H., Sun, D.-W. (2018) 'Multispectral imaging for plant food quality analysis and visualization'. *Comprehensive Reviews in Food Science and Food Safety*, 17(1), 220-239.

Su, W.-H., Sun, D.-W. (2018) 'Fourier Transform infrared and Raman and hyperspectral imaging techniques for quality determinations of powdery foods: a review', *Comprehensive Reviews in Food Science and Food Safety*, 17(1), 104-122.

Su, W.-H., Bakalis, S., Sun, D.-W. (2018) 'Fourier transform mid-infrared-attenuated total reflectance (FTMIR-ATR) microspectroscopy for determining textural property of microwave baked tuber', *Journal of Food Engineering*, 218, 1-13.

Su, W.-H., He, H.-J., Sun, D.-W. (2017) 'Non-destructive and rapid evaluation of staple foods quality by using spectroscopic techniques: a review', *Critical reviews in food science and nutrition*, 57(5), 1039-1051.

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Su, W.-H., Sun, D.-W. (2017) 'Evaluation of spectral imaging for inspection of adulterants in terms of common wheat flour, cassava flour and corn flour in organic Avatar wheat (Triticum spp.) flour', *Journal of Food Engineering*, 200, 59-69.

Su, W.-H., Sun, D.-W. (2017) 'Chemical imaging for measuring the time series variations of tuber dry matter and starch concentration', *Computers and Electronics in Agriculture*, 140, 361-373.

Su, W.-H., Sun, D.-W. (2016) 'Facilitated wavelength selection and model development for rapid determination of the purity of organic spelt flour using spectral imaging', *Talanta*, 155, 347-357.

Jun-Li Xu, BEng, PhD

Project title: A Matlab Tutorial: Performing Dimensionality Reduction in Hyperspectral Image Classification

Project Leader: Prof. Da-Wen Sun

Abstract

This work provides several useful strategies for performing the dimensionality reduction in hyperspectral imaging data, with detailed command line scripts in the Matlab computing language as the supplementary data and it is freely available to be downloaded from: *https://bitbucket.org/lily-xu*. In this work, there are many original codes and functions developed. More importantly, a further selection function based on variance inflation factor (VIF) is proposed to diagnose and alleviate collinearity problem because collinearity and multi-collinearity are always expected to be severe in the spectral data. In this work, step-by-step procedure is provided for easy adaptation of these strategies to individual case.

One effective solution to minimize the collinearity among contiguous wavelengths and avoid singularity is the reduction of data dimensionality. Hence, a reduced image cube can be yielded to take place of the whole hypercube with massive data, and this alteration will remarkably save the subsequent data processing time and will probably enhance model performance in terms of accuracy and robustness. This work is aimed at providing a step-by-step instruction to perform different dimensionality reduction techniques on hyperspectral imaging dataset, with corresponding command line scripts written in Matlab computing language.

In this work, transformation-based methods include principal component analysis (PCA) and linear discriminant analysis (LDA), while band selection methods are comprised of partial least squares (PLS) regression combined with the variable importance in the projection (VIP) scores, selectivity ratio (SR), and significance multivariate correlation (sMC); Monte Carlo sampling (MCS) based methods including enhanced Monte Carlo variable selection (Emcvs) and competitive adaptive reweighted sampling (CARS); model population analysis (MPA) based methods from libPLS including uninformative variable elimination (UVE), random frog (RF), and PHADIA; Matlab built-in functions for feature selection including Relieff, stepwise regression and sequential feature selection (SFS); and the selection method guided by genetic algorithm (GA).

Among all these band selection methods, PLS-based methods (VIP, SR and sMC) have yielded reasonably good classification results. Compared to other band selection methods, PLS-based methods are remarkably simple, reliable and fast. These algorithms work in different manners and they have been designed for various applications. It is thus necessary to conduct trial and error study for finding the optimal one.

Selected Recent Publications

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MODELLING THE KINETICS OF COOKING LOSS DURING POTATO DEHYDRATION USING HYPERSPECTRAL IMAGING

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Abstract

This study assesses the optimal spectral preprocessing methods for modelling cooking loss during potato dehydration using hyperspectral imaging. 6 spectral preprocessing methods combined with 3 regression models are tested. The result shows that SNV is the best preprocessing method for modelling cooking loss. Whereas, the spectra preprocessing method is not useful for Melody potato.

Introduction

The average spectral data extracted from hyperspectral images need to be mathematically improved by spectral preprocessing algorithms before chemometric modelling. In this study, 6 popular spectral preprocessing methods including Exponentially Weighted Moving Average, Savitzky-Golay Smoothing, Extended Multiplicative Scatter Correction, Standard Normal Variate (SNV), orthogonal signal correction (OSC) and Wavelet Transforms (WT) are used to process raw spectral data. Partial Least Squares Regression (PLSR), Principal Components Regression (PCR) and Support Vector Regression (SVR) are then applied to build calibrated models using these processed data. Consequently, optimal preprocessing algorithms for building regression and feature wavelength selection modes will be obtained.

Materials and methods

Sample preparation and experiment set

Cooking loss of the potatoes is measured by weighing before cooking and after cooing. In this experiment, laboratory scale oven is used with the temperature of 80°C for dehydrating potato slices (thickness of 10 mm). The hyperspectral data include four cultivars of potatoes samples (Rooster potato, Cultra potato, Melody potato and Golden potato) obtained at 30min, 60min, 90 min, 150min and 210min during dehydration. There are 12 parallel samples at each time period. Therefore, total 250 samples $(4 \times 5 \times 12)$ are tested at 256 wavelength points in the range from 897.33 to 1752.61 nm (constant interval about 3.33nm). The 4-fold cross validation is used in this study. Therefore, 4 times (folds) modelling will be driven in this research.

All steps described in this study were carried out in the program (see code in **Appendix 1**) written in Matlab R2017b® by the authors.

Select wavelength range

The raw spectra data used in this study shows littery and inaccurate in ranges of start and end spectral bands. The data in wavelength bands which have standard deviation higher than the mean of all standard deviation are dropped. Eventually, the unwanted part has been dropped and the data become more suitable for following modelling.

Exponentially Weighted Moving Average

Exponentially Weighted Moving Average (EWMA) is introduced in this study. The algorithm computes a set of weights and applies these weights to the data samples recursively.

Savitzky-Golay smoothing

Savitzky and Golay (1964) created this simplified method for smoothing and differentiation of spectral data using a least squares technique.

Multiplicative signal correction

Multiplicative Signal Correction (MSC) is also one of the most widely used pre-processing technique for spectral preprocessing.

Standard Normal Variate

Standard Normal Variate (SNV) is a simple and probably the second most applied preprocessing method for scatter correction of spectral data (Rinnan *et al.,* 2009). It can remove both multiplicative and additive interferences of scatter, particle size and the change of light distance (Cen & He, 2007).

Orthogonal signal correction

Orthogonal signal correction (OSC) algorithm is first proposed by Wold *et al.* (1998), they investigated the possibility to remove bilinear components from which are orthogonal to , make a signal correction that does not remove information from .

Discrete Wavelet Transform

Discrete wavelet transform (DWT) is a linear transformation and its trademarks are good compression and denoising of complicated signals and images (Trygg & Wold, 1998). The analyzing mother wavelet used in this paper is the popular Daubechies-4 wavelet function. The spectra are decomposed into five levels by discrete wavelet transform. Then, the detail coefficients vectors are used for reconstruction without using the approximation coefficients vector.

Principle Components Regression

Principal components analysis (PCA) forms a basic multivariate analysis technique for dimensionality reduction and variable selection in spectral data (Wold *et al.,* 1987). Principal component regression (PCR) is a regression analysis technique that is based on PCA. In this study, first 3 principal components are selected according to the cumulative percent of variance explained.

Partial Least Squared Regression

Partial Least Squared Regression (PLSR) does take the response variable into account, and therefore often leads to models that are able to fit the response variable with fewer components. First 3 components have been used to build the PLSR model according to cumulative percent of variance explained.

Support Vector Regression

Support Vector Regression (SVR) is another powerful supervised learning methodology based on the support vector machine (SVM). SVR attempts to minimize the generalized error bound so as to achieve generalized performance (Basak & Patranabis, 2007).

Results

The **Table 1** shows the results of regression models combined with different spectral preprocessing methods. The model SNV+SVR is the best for predicting the cooking loss of Rooster potato, Cultra potato and Golden potato with the RMSE about 0.02734, 0.02953 and 0.2731 respectively. EWMA+PLSR get the lowest RMSE about 0.4368 in predicting Melody potato, whereas, the results are only slight lower than the results obtained by raw spectra. The SVR model get the best prediction results for 3 of 4 potato cultivars, but for other

preprocessing methods, PLSR models get better results than SVR.

Table 1. Root mean square error of prediction results

Preprocessing methods	Regression algorithm	Rooster potato	Cultra potato	Melody potato	Golden potato
Without preprocessing	PCR	0.06905	0.09393	0.07269	0.12384
	PLSR	0.04712	0.05225	0.04368	0.05487
	SVR	0.06027	0.07804	0.05307	0.06321
EWMA	PCR	0.06889	0.09339	0.07285	0.12356
	PLSR	0.04741	0.05256	0.04368	0.05332
	SVR	0.06026	0.07863	0.05309	0.06367
MSC	PCR	0.09009	0.09602	0.05164	0.11397
	PLSR	0.05123	0.05477	0.06239	0.09459
	SVR	0.08001	0.08203	0.05733	0.09566
SNV	PCR	0.03903	0.06522	0.05246	0.06417
	PLSR	0.03114	0.03306	0.05159	0.04072
	SVR	0.02734	0.02953	0.04603	0.02731
Savitzky-Golay Smoothing	PCR	0.06905	0.09392	0.07266	0.12384
	PLSR	0.04715	0.05218	0.04372	0.05497
	SVR	0.06032	0.07791	0.05278	0.06334
OSC	PCR	0.04418	0.06434	0.05286	0.06113
	PLSR	0.03901	0.03499	0.05227	0.03908
	SVR	0.04076	0.03292	0.04772	0.02976
DWT	PCR	0.04701	0.06258	0.05152	0.05836
	PLSR	0.03534	0.04593	0.04719	0.03940
	SVR	0.09085	0.08825	0.06849	0.05279

Conclusion

Using SVR can get robust regression models, and PLSR also has great performance, whereas the PCR is not good for predicting cooking loss. For spectra preprocessing methods, SNV can significantly improve the prediction results, OSC and DWT can also improve the results. However, the spectra preprocessing methods are not suitable for predicting cooking loss of Melody potato. In conclusion, the results of this study can provide a theoretical basis for implementing spectra preprocessing methods in industry.

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EXPOSURE ASSESSMENT OF ACRYLAMIDE FOR IRISH CONSUMERS

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Abstract

Acrylamide in food has the potential to pose significant human risk because of its potential carcinogenic and neurotoxic properties. It is formed as a result of heating starchy foods above 120 °C because of a reaction known as the Maillard reaction. The scope of the study was limited to French Fries, crisps, and coffee from vending machines and the data from literature was used to distil down the exact amount of acrylamide present in these products. The exposure to various demographic groups will be calculated and a Quantitative Risk Assessment model will be generated using Monte Carlo simulation modelling, making use of various scenarios. The Quantitative Risk Assessment model is expected to then tell us whether the exposure is under or over the recommended guidelines.

Introduction

Acrylamide is a chemical substance commonly found in foods such as crisps, bread, coffee etc. It is formed because of a chemical reaction between the natural sugars and the amino acids present in the food substance. The reaction occurs when foods with high starch content are heated to temperatures upwards of 120 °C. Acrylamide can form during all high temperature processes such as baking, frying, roasting (Matthäus and Haase, 2016).

It is assumed that the Irish consumers and the European consumers in general don't come across alarming levels of acrylamide in their diet. So the initial hypothesis is that the human exposure to acrylamide does not pose a significant human health threat to the people living in the Republic of Ireland. The level of acrylamide varies from product to product, and based on the consumption patterns, the exposure to various groups of people tends to vary. Various tools and methods will be used to determine the consumption and in turn exposure levels in three food products: French fries, crisps and coffee from vending machines. **The objective of this study is to develop a risk assessment model to determine the exposure of Irish population to Acrylamide in chosen food products, and to see if it disproves the hypothesis.**

Literature Review

Acrylamide is a chemical contaminant which is associated with heating of starchy foods. It is usually formed as a consequence of Mailard Reaction, which is accompanied by browning of the food surface. It is a class 2a carcinogen (Hamzalıoğlu *et al.* 2018) with known effects on developmental properties of the brain.

A study (Mesías and Morales 2016) tried to evaluate the levels of acrylamide in brewed coffee acquired from vending machines. The paper was aimed at the Spanish population, but the results can be assumed to be generally true for all European/ Irish consumers as well. The level of acrylamide found in vending machine coffee ranged from 7.7 to 40.0 µg/L. It was found that the levels were not affected by the extraction procedures. Dietary exposure was estimated at around 0.037 µg/kg body weight per day. Since the lowest No Observed Adverse Effect Level (NOAEL) is 0.2, it was concluded that coffee from vending machine does not pose a significant health risk for Irish/European consumers.

A paper (Cummins *et al.* 2008) used a farm to fork exposure assessment model to determine the levels of acrylamide in fried potato crisps for Irish consumers. The paper modelled different stages in the production of crisps such as potato production, storage, crisps production, and finally consumption. Mean level of acrylamide in fried potato crisps was found to be 720 µg/kg and exposure was estimated to be 0.052 and 0.064 µg/kg/bw/day for males and females respectively. According to the paper (Medeiros Vinci *et al.* 2012), the mean levels of acrylamide in French Fries were found to be 159 to 963 µg/kg.

Methodology

Model

For a typical person, food is one of the major sources of acrylamide. The main food products to be included in the assessment were determined to be French fries, potato crisps and coffee from vending machines, as these products are major contributors in an Irish diet. According to the WHO, the general intake of acrylamide is in the range of 0.3 to 0.8 microgram per kilogram of body weight (Hogervorst *et al.* 2007).

The likely levels of acrylamide in the products were distilled from the literature, as defined in the literature overview. Using survey tools such as Irish Universities Nutritional Alliance (IUNA) and Safe Food (Food), consumption patterns for both males and females were analyzed. Nutritional surveys in IUNA, for example, were divided according to surveys conducted among various demographics such as preschool children (NPNS), teens (NTFS), adults (NANS) and children (NCFS). (IUNA 1997-2018). Exposure was measured in µg/kg/bodyweight/day, level in µg/kg per population studied, and consumption was measured in µg/kg/bodyweight. The calculation involved in the study was based on:

Exposure = Level of Acrylamide in food × Quantity food Consumed

Data from the sources above will be used in the RASP system. Monte Carlo simulation will be run with no. of iterations set to 1000 and bins set to 10 (Mahadevan 1997).

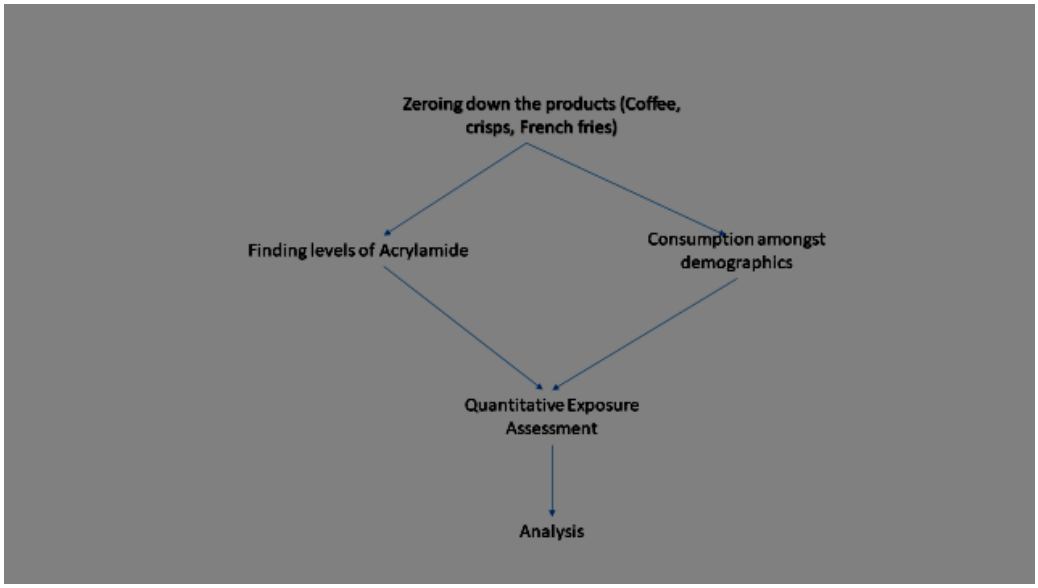

Figure 1. Proposed steps in the study

Analysis

According to WHO guidelines, human exposure should not ideally exceed 1µg/kg body weight per day with a maximum level set at 4 µg/kg body weight per day (WHO 2002). After the characterization, the exposure concentrations will be checked to see if they conform to these and the EU/National regulatory guidelines. The probable mitigation strategies can then

be devised based on the difference in impact of the various inputs to the Quantitative Risk Assessment model, and other forms of scenario analysis. The final results will be presented in the form of a probability density versus acrylamide exposure curve graph.

Conclusions

Studies are continuously being done to determine the exact nature of the effect dietary acrylamide can have on humans. It is a potential carcinogen so consumption of products such as coffee, crisps and French fries should be reduced, and steps should be taken to reduce the levels in the products by understanding how it's formed during the cooking process. The scenario analysis can help pinpoint the relationship between acrylamide and various factors leading to its formation. The results of the exposure assessment model will show whether a typical Irish consumer is at risk from consumption of these products by comparing the exposure against the guidelines set by WHO and other regulatory bodies (WHO 2002).

Acknowledgements

The author wishes to thank his peers for their constant encouragement and support.

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PRELIMINARY QUANTITATIVE RISK ASSESSMENT OF SALMONELLA IN IRISH CHICKEN BREASTS FROM RETAIL TO CONSUMPTION

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Abstract

The current quantitative risk assessment model will aim to estimate the possible risk of human salmonellosis which may occur due to consumption of chicken breasts bought from Irish superstores and cooked in Irish home kitchens. The model will virtually simulate the level of *Salmonella* contained on chicken breasts from the retail to table pathway. Irish parameter values will be used for data input, where available, to represent risk of salmonellosis. Variation in the population of *Salmonella* on each chicken breast will be simulated using the assistance of growth and inactivation equations. The results from this model will emphasise the shared responsibility of various parties involved from retail to table for protection from *Salmonella.*

Introduction

Salmonellosis is one of the most frequently reported food borne illnesses in Ireland. In Ireland, 333 cases of salmonellosis (1 of these cases was not laboratory confirmed) were reported to the HPSC in 2009, corresponding to a crude incidence rate (CIR) of 7.9 cases per 100,000 population. Preventing outbreaks of salmonellosis from chicken needs a collective approach to chicken safety. One such holistic approach is risk assessment, which consists of hazard identification, exposure assessment, dose–response assessment, and risk characterization. The usual approach taken is to construct a quantitative risk assessment model (QRAM) in a computer spreadsheet using probability distributions to model the variability and uncertainty of important risk factors, such as time, temperature and pathogen density. The QRAM is then simulated using a spreadsheet add-in program that randomly samples the probability distributions and uses the random numbers generated to perform calculations and generate output distributions (Vose, 1998).

Risk Assessment Framework

Microbial risk assessment is a step by step method for testing the nature and extent of risk related with a microbe caused hazard in a food product, provides a framework: (i) to identify potential risk elements related to the predicted risk, (ii) to weigh and select the most suitable mitigation plans to reduce this risk, and then (iii) to provide important information based on the results to the decision making process.

The conclusion of the risk assessment method is intended to provide filtered and concise information to inform decision making related to public health. The main aim of the model that will be used will be to approximately calculate the risk of salmonellosis due to consumption of chicken breast containing salmonella by considering: (i) the probability of undercooking and (ii) the probability of post cooking cross contamination in Irish kitchens. For each of these scenarios, *Salmonella* concentration will be an output that will act as an input into the next step in the modeling process. The estimation of dosage will be used to predict the probability of salmonellosis per year due to the consumption of *Salmonella* on chicken breast bought from retail stores, and consumed by the locals. The chain of focus is the retail to consumption pathway considering origin of contamination at various stages along the chain and their successive effect on human health.

A framework model to conduct an exposure assessment is depicted in the following Fig.1

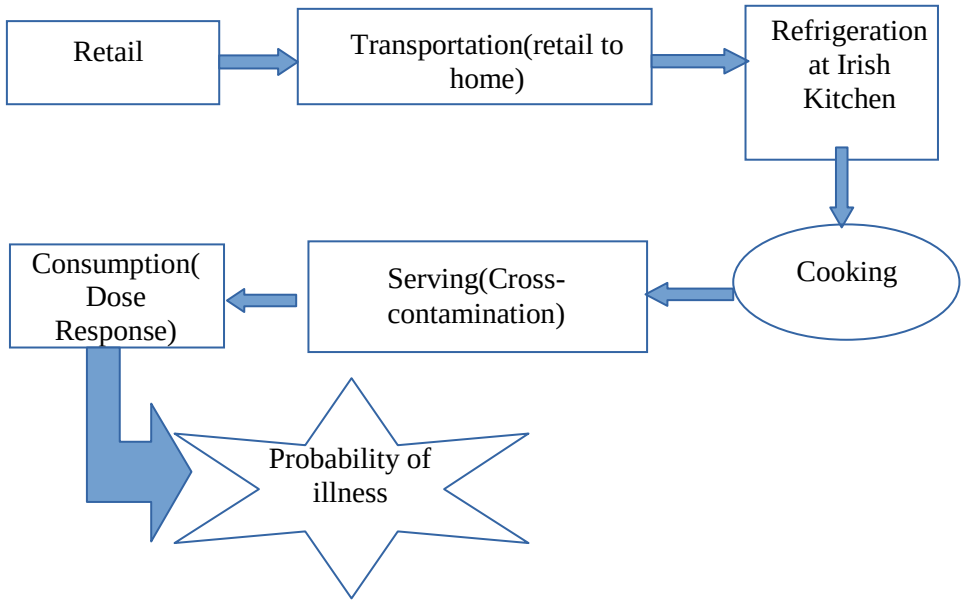

Fig 1. Flow diagram model for risk assessment of Salmonella in Irish Chicken breasts.

Methodology

A QRAM will be developed for Salmonella and chicken breast that uses Monte Carlo simulation methods to model the effects of initial contamination after processing, growth during distribution, thermal inactivation during cooking, cross-contamination during serving and host resistance on the probability of salmonellosis.

Ten thousand iterations will be performed in order to increase the reliability of the software to reproduce the defined distributions. Every iteration will depict a randomly chosen chicken breast from the retail store going through various steps finally being consumed at Irish homes. The outcome of the result will be: contaminated if it is above the set value or not contaminated if it is not above the set value.

Quantitative information required for different stages will be gathered through a literature search to identify all potential relevant research including peer-review articles, national surveillance reports, epidemiological surveys, industrial surveys, governmental reports, and unpublished research work. Relevant screening will be conducted for all collected abstracts for each stage from retail to consumption identified within that stage. The resulting data will be then summarized and pooled.

Data Analysis

The data will be analyzed by plugging different input settings using the PERT distribution which will have three parametric values for the graph in the distribution for various stages at Retail, Consumer Transport(Time), Cooking(Temperature), Serving and Consumption. The input values will range from 0-100%. PERT when combined with MPN(Most Probable Number) will give a flexible shape which varies from a normal distribution to a log normal distribution that is skewed to the right or left. Statistical methods will be employed using Monte Carlo plug-in on Excel spreadsheets and relevant graphs for finding hot spots along the retail-consumption chain will be plotted along with prevalence graphs, related tables and charts.

Expected Results

Exposure assessment results will be obtained after the consumption stage where response for the consumption event will be modeled as a discrete event where illness did not occur if the amount consumed was less than the positive exposure limit, whereas illness occurred if the amount consumed was equal to or greater than the exposure limit.

The results obtained through the QRAM should be in agreement with the epidemiological data and finally conclusions will be drawn based on the assessments by comparing different stages along the chain keeping in mind various influencing factors like time, temperature and handling methods which may indicate hot spots.

Conclusions

Quantitative risk assessment modeling is a holistic approach that has a great potential as a decision analysis tool for the chicken industry. This model utilises existing data to check the changes in salmonella population from retail to table pathway and can be used as a risk management tool and divert focus towards critical steps along the retail-consumption chain. *Salmonella* can be controlled by the food handlers at retail and in private kitchens.

Acknowledgements

This research paper was completed with the support of my peers who provided insight and expertise that greatly assisted the research.

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RISK ASSESSMENT OF NOROVIRUSES IN FOOD

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Abstract

Norovirus contaminated shellfish pose a significant threat to consumers' health. It is considered as a possible source of foodborne illness when eaten in raw. As filter feeders, when living in an environment polluted with human fecal material, a large number of Noroviruses can be detected from the oysters. Oyster norovirus outbreaks, apart from showing a seasonal trend, are also influenced by other factors. In this study, the geographic factor was identified by using publically available data. The numerical data were collected from peer-revived journal articles, mainly focusing on the data addressing the oyster contamination issues in Europe, and in China. Then, the data were processed with Excel for further analysis. The result shows that time of year and sea temperature has an impact on the oyster contamination levels; more positive oyster samples can be detected from total samples with lower sea temperature.

Introduction

Norovirus (Nov) is the most common cause of non-viral gastroenteritis (Baldridge *et al.*, 2016). According to official reports, there are around 23 million cases of severe gastroenteritis with the infection of Nov, symptomatically performed acute-onset vomiting, watery non-bloody diarrhea with abdominal cramps, and nausea. In the meantime, those infected people could excrete millions of viral particles in faeces that is very likely disseminating to the air and water system without proper wastewater treatment and effective inactivation method (Gentry *et al.,* 2009). The faecal-oral route is a typical transmission pathway via contaminated surfaces, food, water or even by person-to-person spread (Baldridge *et al.,* 2016).

The consumption of shellfish is considered a possible food source of norovirus infections. As bivalve shellfish are filter feeding, they concentrate those microorganisms existing in the water. When living in the norovirus contaminated water system, a high concentration of viruses could be detected from the shellfish. More importantly, most of the bivalves, such as oyster, mussel, and scallops are often served and eaten raw, leading to the viral gastroenteritis outbreaks. Based on epidemic studies, Nov caused foodborne outbreaks present a seasonal pattern, showing a high risk of infection when consuming oyster in the winter (Lowther *et al.*, 2008). From October to March, a high level of noroviruses in oyster could be identified (Lowther *et al.*, 2008).

Apart from winter seasonality, the level of Nov existing in the shellfish is also driven by other factors. According to recent research conducted by Strubbia *et al.* (2016), Nov concentrations are also influenced by the location of harvest site. For the place near to sewage, a higher concentration of Nov is observed in the oysters (Strubbia *et al.,* 2016). Therefore, it is assumed that geographic factors could have an influence on the contamination levels of Nov in oysters.

The objective of this project is to determine the geographic factors affecting the concentration of Noroviruses in oysters.

Materials and Methods

Data collection and processing

This risk assessment project was achieved with secondary data from publicly available sources. The numerical datasets were collected from peer-reviewed journal articles via the different database, mainly focusing on the dataset addressing the oyster contamination problems in Europe, and in China. To obtain more relevant and specific data resources, key words were used during searching, including 'Noroviruses contamination', 'oysters', 'outbreaks' and 'harvesting sites'. Currently, three datasets were employed (details are shown in Table 1.), of which oyster samples were collected from the harvesting site monthly.

The Global Sea Temperature website (https://www.seatemperature.org/) was used for collection of monthly data for seawater temperature, including maximum and minimum. The value used in this study is the mean sea temperature.

Table 1. Information about the datasets used in this project

Harvesting site	Investigation period	Reference source
Ireland	Aug. 2006 - Jul. 2007	Keaveney *et al.*, 2007
France	Feb.2010 - May.2011	Schaeffer *et al.*, 2013
China	Sep. 2015 - Sep.2016	Tao *et al.*, 2018

Data analysis

The datasets were put into the Microsoft Excel and managed for further data analysis.

Results and Discussion

The occurrence of Norovirus shows a similar trend not only in the European countries (Figure.1 and 2) but also in China (Figure 3). The sea temperature is inversely proportional to the oyster contamination level. For instance, the colder the seawater, the higher frequency of positive samples can be identified. During winter time, when the sea temperature is the lowest, the ratio of positives to the total oyster samples is the highest, which indicates the peak of oyster Norovirus outbreaks.

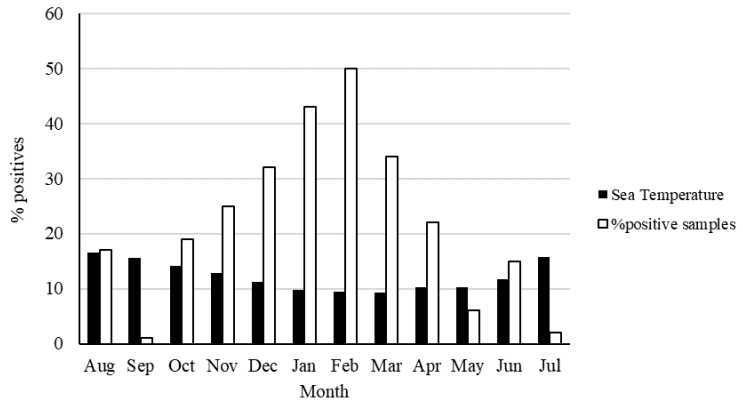

Figure 1. Variation of positive oyster samples affected by sea temperature in Ireland

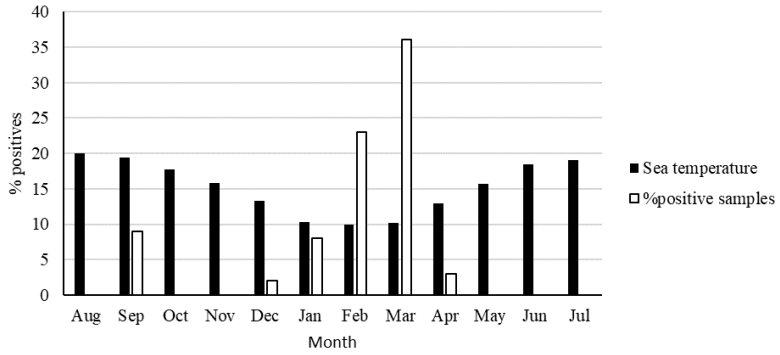

Figure 2. Variation of positive oyster samples affected by sea temperature in France

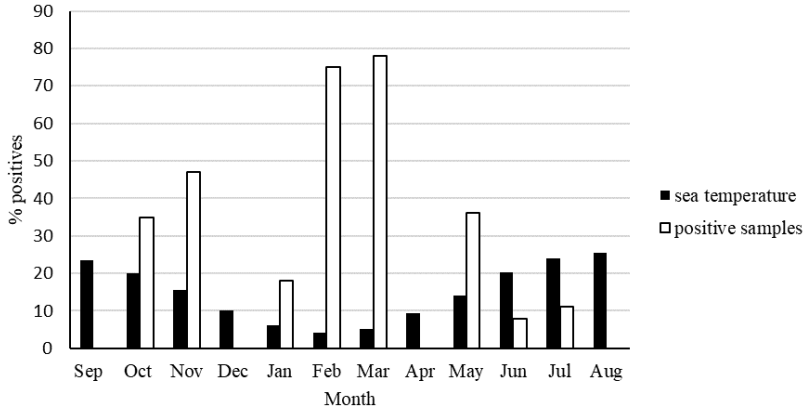

Figure 3. Variation of positive oyster samples affected by sea temperature in China

Conclusion

The number of norovirus-contaminated oysters is higher with lower sea temperature. This indicated that in winter when the seawater temperature is relatively low, oysters tend to be less active. So, they expel the viruses less quickly. This is also the time of year when the number of human cases is at its highest, so that contamination of sea water is at its highest during the winter months.

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RISK ASSESSMENT OF MICRO PLASTICS IN FOOD CHAIN

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Abstract

In today's world the pollution of water sources by micro plastics is a topic of global concern. These plastics eventually end up in the ocean and pollution of oceans by plastics represents a major environment problem. Until now research conducted and literature available on the interaction of microplastics in the ocean, within the aquatic organism and the risk arising from the ingestion of these seafood in humans is limited. Microplastics have been found in various foods such as beer, honey and salt. To determine the occurrence of microplastics in human seafood is the major challenge. This study will develop a model to examine different aquatic species potentially ingesting microplastics and its potential impacts on human health as a result of secondary microplastics consumption. The model is based on number of different investigations testing the concentration of plastics and rate of ingestion of these hazards within the animal gut as most of microplastics will be present in the GI tract of the marine organisms.

Introduction

The production of plastic is increasing at a tremendous rate since early 1950 and a report suggested that the global plastic production reached 335 million in 2016 and is expected to reach 600 million by 2025. Microplastics are defined as plastic particles ranging from 0.001 micrometers to 0.11 micrometers.

The major source of marine pollution is plastic accumulation and debris. Plastics comprise the largest part of marine debris and have been reported as important pollutants in marine as well as fresh- water environments (*Thompson et al., 2004; Cole et al., 2011; Maximenko et al., 2012; Wagner et al., 2014*). The most common exposure pathway of microplastics is by ingestion and its reported in 270 different taxonomies and marine organisms which are mostly affected. According to a study conducted in 2006 by *Allsopp et al.* roughly 4.6% of all plastic produced ends up in oceans, while another study by *Barnes et al. (2009*) estimated that around 10% of global plastic production ends up in oceans. A recent study by *Eriksen et al., (2014)* revealed that the ocean contains an estimated 5.35 trillion particles of plastic in which microplastics comprises around 92.4%. Most of the microplastics ingested by the organisms are present in the gut of the organism and for human consumption the gut is removed so there are less chances of exposure from microplastics by humans. The ingestion of plastics by marine organisms can be harmful for the organism and can affect their metabolic processes and interfere with their immune system. These can then have an impact on human health when consumed as seafood as the plastic and its chemicals tends to accumulate in the tissue. Humans are potentially exposed to these contaminants through bioaccumulation and biomagnification in the food chain.

The objective of this study is to develop an exposure model to determine the presence of microplastics in seafood and resulting risk associated with the consumption of this food for humans.

Methodology

The methodology will be to collect and analyze the data from the literature available and develop the model for different stages of the risk assessment process. The first step will be to determine the levels of plastic entering the oceans from different sources. The next step will be to identify the percent of plastic ingested by fish and other aquatic species and the amount of plastic present in the tissues of these aquatic species and to analyze the risk of plastic exposure on the aquatic organisms. As seafood is the major source of microplastic contamination in the human diet the next step will be to determine the intake levels of seafood consumed by different individuals and the amount of plastic being ingested in the form of seafood. The next step will be to combine the data and develop a model which will help to examine the levels of plastic in the oceans and the risk associated with the consumption of seafood on the human health. A framework model is presented within which the risk associated with micro plastics in sea food can be determined:

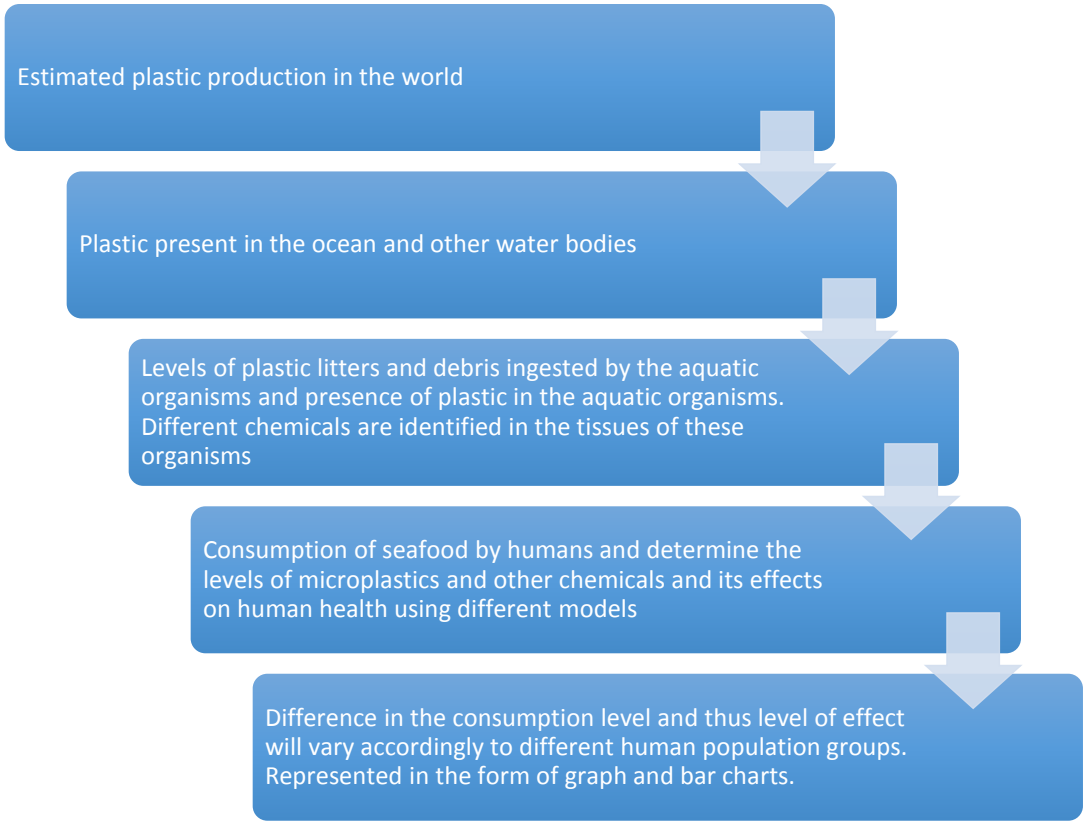

Figure 1: framework model for risk assessment of micro plastics in sea food.

Result

According to the literature reviewed and data collected and analysed, microplastics are present in almost all the species of fish and other organisms. Mostly the microplastic present will be in the gastrointestinal tract of the organism. This shows that microplastic has an effect on the marine organisms. The result also proves that seafood when consumed, a small percent of microplastic is being consumed by the human as a form of secondary consumption of microplastic. On average, humans consume some amount of microplastic through the food chain while studies suggest the packaging method impacts the source of microplastic contamination. The presence of microplastics is being documented worldwide in water-

column and sediment samples, and their presence has also been reported in different taxa including planktonic species, in- vertebrates, fish and cetaceans (*Browne et al., 2011; Hidalgo-Ruz et al., 2012; Foekema et al., 2013; Lusher et al., 2013, 2015; Van Cauwenberghe et al., 2014, 2015a).*

Conclusion

Contamination of microplastics is possible through seafood, as seafood can be contaminated by microplastics not only through environment but also through food packaging and food processing. Microplastics contamination not only represent physical risk but also chemical and biological risk. This study, found that microplastics are present in different species of fish and other marine organisms. The study also concludes that most of the microplastics are present in the stomach and intestine of the fish. It is also predicted that fish can be a source of PBT dioxins and the level of these PBT is found to be higher in humans consuming high amounts of seafood as compared to the population consuming a lesser amount. Knowledge on the effects of microplastics is still very limited and more research needs to be carried for the presence of microplastic and its effects after consumption.

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DIETARY EXPOSURE ASSESSMENT FOR ARSENIC IN RICE

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Abstract

Rice as a staple food worldwide contains higher arsenic than other crops, it has been one of potential concerns to human health. High arsenic in rice may cause series of diseases and even cancers. More research should be performed to uncover the dietary exposure of arsenic based on daily rice consumption. This study evaluated the arsenic exposure in seven typical countries based on rice consumption. An exposure assessment model was developed to quantify the arsenic exposure using the RASP simulation software. The preliminary results showed that arsenic exposure from rice consumption was the highest for Bangladeshi with mean exposure 1.51 μg/kg per day, this might be correlated to high rice consumption. In Bangladesh, 95% of consumers were exposed to under 2.61 μg/kg per day, while in France, 95% of consumers had an extremely low exposure with only 0.09 μg/kg per day. Comparing the exposure level to regulations by WHO and EFSA, the exposure level of arsenic in all counties investigated are under the limit. The model developed might be helpful to rice-staple countries in evaluating exposure to arsenic.

Introduction

Arsenic (As), which is found in several different chemical forms and oxidation states (−3, 0, +3, +5), causes acute and chronic adverse health effects, including cancer (Michael, 2002). It has been detected in water, soil and air from natural and anthropogenic sources. Over the past two or three decades, occurrence of high concentrations of arsenic in drinking-water has been recognised as a major public-health concern in several parts of the world (Mukherjee *et al*., 2006). However, recently it was found that As is also accumulated in food crops especially in rice (Islam *et al*., 2016). Rice is an essential staple food and feeds over half of the world's population, such as in India, China, parts of South America and South East Asia (Conway and Toenniessen, 1999). Consumption of rice has increased from limited intake in Western countries some 50 years ago to major dietary intake now.

Rice contains about ten times more As than other crops, it was mostly reported that arsenic concentrations in rice were found in the range from 0.02 to 0.90 mg kg^{-1} (Meharg and Zhao, 2012) and As in rice grains was usually below 1.0 mg kg^{-1}(Rahman *et al*., 2009). There is evidence indicating that rice consumption represents a major route for inorganic arsenic exposure in many countries, especially for people with a large proportion of rice in their daily diet as much as 60% (Islam *et al*., 2016) and high arsenic in rice is associated with elevated genotoxic effects in humans which cause alterations in immunological, gastrointestinal, hematological, pulmonary, cardiovascular, neurological, and reproductive/developmental function (Banerjee *et al*., 2013). Thus, worldwide Arsenic in rice is a serious concern for > 3 billion people across the world who consume rice as a staple food and millions of people may be at risk of developing As-related health problem. However, total As concentration in rice varies widely depending on the cultivar of rice and the place where it was cultivated. Some factors such as soil, fertilizer, irrigation, and rice genotype influence the arsenic concentration in rice. It results in geographical variation in arsenic content of rice. Meanwhile, rice average consumption in different regions around the world has a big difference because of consumption practice.

The objective of this study was to quantify dietary exposure of arsenic in rice and assess potential health implications arising.

Materials and method

Exposure assessment is an essential approach for quantifying risk. Dietary exposure assessment combines food consumption data with data on the concentration of specific chemicals in food. The resulting dietary exposure estimate may then be compared with the relevant health-based guidance value for the food chemical of concern, if available, as part of the risk characterization (World Health Organization, 2009). In this case study, we need to access data including rice consumption, arsenic content in rice and average body weight for exposure assessment.

Data inputs and developed model

Rice consumption

According to the report from OECD/Food and Agriculture Organization of the United Nations (2015), daily rice consumption per person is among the highest in Asia, reporting rice intake exceeds 300 g per capita per day, China and India consume approximate 50% of total rice consumption of the world. Specifically, as shown in table 1, the average rice consumption Bangladesh, China, Japan and Thailand were 464, 209, 155, 390 g/day/person. Egypt also had high consumption of rice, average consumption of rice is about 114 g per capita per day. In countries such as France, which was selected to represent EU, its rice consumption had the lowest level among the countries, just 13 g per day per capita, while in USA, the consumption of rice has increased rapidly, averaging about 34 g per day per capita.

Arsenic content in Rice

The arsenic content in rice was summarized by Meharg *et al*., (2006) it shows that Egyptian rice had the lowest mean arsenic concentration at 0.05 mg kg^{-1}, followed by Bangladesh (0.13 mg/kg), Thailand (0.13 mg.kg), China (0.14 mg/kg), Japan (0.19 mg/kg), USA (0.25 mg/kg) and France (0.28 mg/kg). The arsenic concentration among the seven countries had a wide range determined by rice types and locations, specific data were shown in table 1.

Average body weight

As shown in table 1, the average body weight in the countries investigated was collected from the report by Quilty-Harper, in (2012).

Table 1: Arsenic content in rice, average rice consumption and average body weight in typical counties of the wold

Countries	Total As		Rice consumption	Body weight
	Range (mg kg^{-1})	Mean (mg kg^{-1})	(g/day)	(kg)
Bangladesh	0.02 – 0.33	0.13	464	49.59
China	0.02 – 0.46	0.14	209	60.56
Egypt	0.01 – 0.58	0.05	114	74.27
France	0.09 – 0.56	0.28	13	66.78
Japan	0.07 – 0.42	0.19	155	59.02
Thailand	0.01 – 0.39	0.14	390	58.79
USA	0.03 – 0.66	0.25	34	81.93

The amount of arsenic exposure to human was estimated by following equation:

$$HE = AC \times RC/bw$$

Where HE is human exposure to arsenic (µg/kg/day), AC is arsenic content in rice (mg/kg), RC is rice consumption (g/day) and bw is body weight (kg).

Results and discussion

The preliminary results for human exposure to arsenic in rice using the RASP simulation modelling system show that arsenic exposure from rice consumption was the highest for Bangladeshi with mean exposure 1.51 μg/kg per day, this was followed by Thailand (1.22 μg/kg per day), China (0.71 μg/kg per day), Japan (0.58 μg/kg per day), Egypt (0.33 μg/kg per day), USA (0.13 μg/kg per day) and France (0.06 μg/kg per day). Although arsenic content in rice is one of key factors to determine exposure level, the arsenic exposure in most of countries correlates well to amount of rice consumption. Rice consumption might be the most important factor influencing the exposure level.

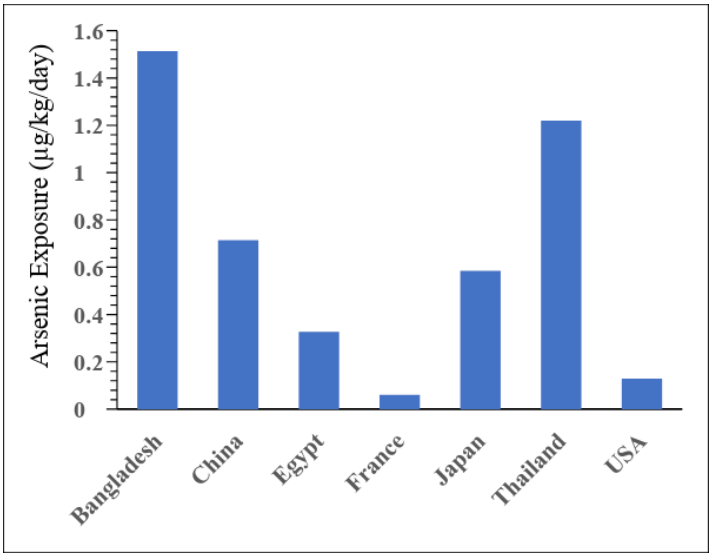

Figure 1: Preliminary simulated results for human exposure to arsenic

At confidence level 0.95, the value of arsenic exposure was calculated by the RASP simulation modelling system. In Bangladesh, 95% people was under 2.61 μg/kg per day, while in France, 95% people was exposure to an extremely low level with only 0.09 μg/kg per day based on rice consumption.

Table 2 Arsenic exposure (μg/kg per day) in different countries at 0.95 confidence level

Confidence Level	Bangladesh	China	Egypt	France	Japan	Thailand	USA
0.95	2.61	1.31	0.72	0.09	0.91	2.13	0.23

Based on a 0.5% increase in prevalence of lung cancer, JFAO of UN and WHO determined a lower limit that was 3.0 mg/kg body weight per day. As well, a report from EFSA showed that dietary exposure level of arsenic (0.13 to 0.56 mg/kg body weight per day) in food and water is within range of the proposed BMDL values, indicating that the risk induced by toxicity of arsenic in food and drink cannot be neglected (EFSA, 2009). When comparing the exposure level to regulations, obviously, the exposure level of arsenic in all counties investigated are under the limit. But the risk induced by toxicity of arsenic in food and drink cannot be neglected because the long-term intake might increase the prevalence of diseases related to arsenic toxicity.

Conclusions

This study was performed to assess the arsenic exposure in typical regions based in daily rice consumption. The arsenic content in rice and rice consumption within the regions investigated were

collected from Journal articles and reports by WHO. A simple exposure assessment model was developed to quantify the arsenic exposure using the RASP simulation software. Preliminary arsenic exposure caused by rice consumption was estimated in seven typical countries. The results showed that arsenic exposure from rice consumption was the highest for Bangladeshi with mean exposure 1.51 μg/kg per day, this might be correlated to high rice consumption. In other countries, such as China and Thailand, arsenic exposure from rice consumption also kept at relatively high level. In Bangladesh, 95% of consumers was under 2.61 μg/kg per day, while in France, 95% of consumers were at an extremely low level with only 0.09 μg/kg per day. Although comparing the exposure level to regulations by WHO and EFSA, exposure level in all countries are far below the limit, but the risk still cannot be neglected because of the long-term rice intake and arsenic accumulation within human body. The correlation between arsenic exposure from rice consumption and diseases related to arsenic toxicity should be studied.

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Rajat Nag, BE, MSc

Project Title: The comparative public and animal health risks associated with spreading Anaerobic Digestate.

Project Supervisor: Assoc. Prof. Enda Cummins

Abstract

Anaerobic Digestion (AD) is a biological process which utilizes the organic waste to produce biogas (Methane) which can be further used to generate heat and electricity. The digestate which is a co-product of the process contains essential nutrients and it can be used as organic fertiliser. At the same time, the volume of food and animal waste can be reduced so that a minimum amount of waste can be landfilled. However, farmyard manure and slurry (FYM&S) and digestate contain a huge number of harmful pathogens (bacteria, fungi, viruses, parasites). Once the FYM&S and digestate are spread on land, the pathogens can be transported through environmental pathways. The objective of this study was to evaluate the human and animal risk associated with spreading FYM&S and anaerobic digestate on land with the help of qualitative and quantitative risk assessment models. Risk assessment is comprised of four sections such as a) hazard identification, b) exposure assessment, c) hazard characterisation and d) risk characterisation. The Hazard identification task has been completed selecting 99 pathogens from outbreak data and consulting with the literature published by EU commission on the possible presence of pathogens in anaerobic digestate. A simple qualitative scoring system was developed based on likelihood and severity of illness. The target pathogens are identified from the screening model. A qualitative scoring system was used to categorise (i) inactivation status following heat treatment (score S1) (ii) hazard pathway (score S2) and (iii) severity (score S3). The S1 score was introduced to consider the effect of thermal inactivation for the mesophilic and thermophilic AD process conditions and possible pasteurisation regimes. The S2 score focused on the number of potential pathways of transmission (e.g. bio-aerosols, water, soil, through food and zoonotic contact). The severity of potential illness was computed by the S3 score considering any previously reported outbreak and mortality data. The final Hazard Screening Score (S-Score) was computed as the product of the individual S1, S2 and S3 scores for the pathogen. The final S-Score can be used to scientifically rank potential biological hazards from the AD process which may be present in the resulting digestate and allowing for prioritisation and further detailed risk analysis of the hazards of potential health concern. The overall study will fill the gaps in the literature finding out the sources of pathogens in the raw materials of the AD, the mesophilic and thermophilic effect in pathogen inactivation, the influence of pasteurisation, available strategies for risk assessment and connection with the EU and Irish legislation. Furthermore, risk assessment in this area will improve our understanding regarding the most critical parameters such as; temperature (mesophilic or thermophilic), pH, organic loading rate, Carbon: Nitrogen ratio and hydraulic retention time of the AD process including the scenarios of different feedstock recipes, with or without pasteurisation, pre or post pasteurisation, and finally the effect of storage on pathogen lethality in relation to minimize the biological risk.

Yingzhu Li, BE, M.EngSc., PhD

Project Title: Human health risks from engineered nanoparticles

Project Leader: Assoc. Prof. Enda Cummins

Abstract

In the last decade, nanoparticle induced toxic endpoints have been revealed for many species, some of which may exceed human exposure limits. There are many gaps to fill in order to complete a whole risk assessment for engineered nanoparticles (ENPs). Black boxes are typically used to model fate in environmental medias, and the sophisticated toxic mechanism. Therefore, this project aims to establish a comprehensive model to evaluate nanoparticles' risks, and human health risks. Various methods are adopted to identify central issues. Systematical review methods such as meta-analysis are used for identifying the specific question underlying the nano-toxicity acting mechanisms on different species and cell lines. The behavior kinetics in natural waters under various environmental conditions are of concern. A risk assessment of selected nanoparticles is being established by employing quantitative data. A quantitative risk ranking is being conducted. Dose-response curves selected from animal testing and a benchmark dose modelling approach is being developed to compare nanoparticles in terms of impacts on human health. A literature review on health impacts from silver nanoparticles (AgNPs), identified lungs and kidneys as the major targets for mammalian animals. A series of prolonged damage had been revealed through various testing methods from gene level to organ level. Subchronic toxicity was revealed on rats through oral uptake of AgNPs with average particle size at around 20 nm. Due to the variety of sizes and other surface properties, more in vivo tests are necessary in studying nano-specific toxicity, or, conduct a risk assessing model to encode these properties. By solving control issues listed above, both the frame and data platform of a risk assessment model will be compiled.

Qicheng Hao, PhD

Project Title: Occurrence of Cronobacter in a dairy powder ingredient plant

Project Leader: Prof. Francis Butler

Abstract

Cronobacter is a kind of bacterium which ubiquitously in environment and food. It has high ability of alive even in a dry area. There shows that it has less harm for adult but much more dangerous to new born babies. This research is focus on the environment of dairy powder manufactory which may cause the contamination of the final products.

The process of pasteurization in milk powder manufactory can sterilize Cronobacter. Processes of dry and packaging which are after pasteurization will be the locations to pick samples. The bacterium isolated form these areas will be sequenced to find out contamination sources.

The first step is surveillance programme. Sampling of swabs from milk powder environment that occurred over a twelve-month period, once a month. These swab samples were taken from twenty locations of the processes of dry and packaging. The locations include the surface of equipment, wall, ground, ventilation system and other points which may contaminated. Then samples were tested for Cronobacter spp. in accordance to the updated ISO method. For next step, DNA of positive samples were extracted for sequencing and strains were also stocked to -80℃ for future record. The sequencing data was analysed buy programme of pipeline to identify the gene type for sources analysis.

Eighty-eight positive samples were isolated for 250 samples. Four gene types were identified which are ST1, ST4, ST41, ST42. The isolation result shows that the worst months are spring and autumn. That may because in summer time, the environment is to dry for cronobacter to grow. In June and July, only one positive result was got out of the twenty locations. For the locations, the most positive were got is from location 5 and 6. That may because these areas are wet and warm which is suitable for cronobacter. The result form sequencing shows that ST4, which is associated to infant infections, was the lowest frequency appeared. That means there is not just one source of contamination, but the most dangerous strain was well obstructed.

For conclusion, sequencing indicates multiple contamination sources. Surveillance work in conjunction with sequencing identified a ‘hot spot’ of contamination for ST1, 41 and 42. For further work, an intervention study to assess deep cleaning of contaminated areas will be looked at. Further work will also look at if there are different strains in the same location.

RISK ASSESSMENT OF PORK PRODUCTS PRODUCED IN CHINA

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Abstract

Salmonella is derived from livestock especially in raw pork or pork products and it is a cause of foodborne illness. To reduce the cases of illness caused by Salmonella, a quantitative microbiological risk assessment (QMRA) was used to assess the different points in the farm to fork chain of pork products. (Vigre *et al*., 2016) The present study of Salmonella in China collects data on Salmonella distribution from farm to fork chain of pork products and reveals that cross-contamination of Salmonella occurs at different sites. All this data can give suggestions for the control Salmonella. (Zhou *et al*., 2017)

Introduction

Salmonella is one of the critical foodborne pathogenic bacteria in the world. It is commonly isolated from raw pork and is a leading cause of foodborne illness. In China, approximately 70%-80% of foodborne pathogenic outbreaks are caused by Salmonella (LI *et al*., 2014). livestock and pigs are considered to be the major carrier of Salmonella and pork has been identified as one of the most frequently contaminated meats.

Pork is most important sources of meat in Chinese daily life due to the price of pork is cheap and acceptable compared with other meat like beef showing in the following graph. (USDA, 2018) Also, IATP (2017) analyze that China's emergence as the largest producer and consumer of pork in the world. In 2017, China has become the biggest pork importer in the world. However, there are no thinking about that in lots of poor places in China, and people do not consider the origin, quality of meat and whether or not these were contaminated. This is a potential risk for the health of people. So through study of Salmonella to built proper estimate system and make risk assessment of Salmonella have important meaning in China.

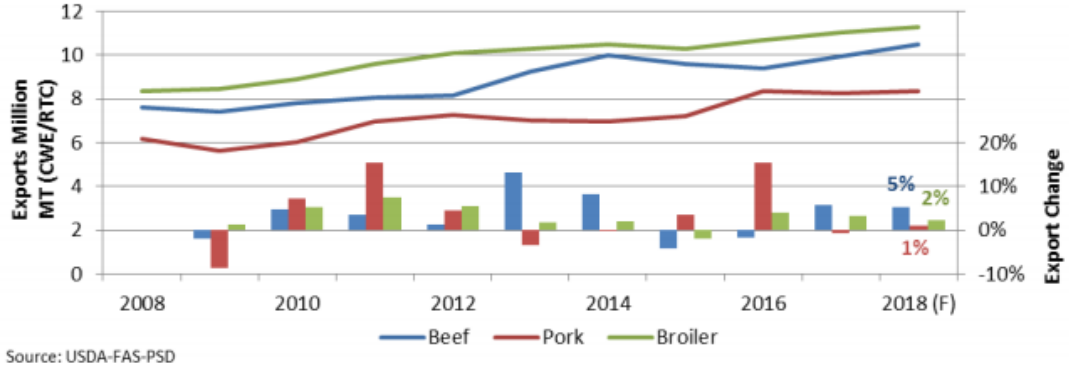

Figure 1: Exports of meat products

The aim of the study is to use a quantitative microbiological risk assessment (QMRA) in the farm to folk chain using data from China.

Materials and Methods

Data collection

Jiangsu is a near sea province in the eastern portion of China and has a population of 70 million and is the region where most of the pork is produced. (Li *et al*., 2014) So the data collected from here is meaningful in a Salmonella study from the farm to fork chain in China.

Through an exposure assessment of Salmonella isolates, a Salmonella samples distribution can be developed which provides a quantitative insight. These data are the basis of a QMRA to control Salmonella in different processing from farm to fork.

Data analysis

Data on the prevalence of Salmonella from different provinces include Nanjing, Yangzhou, Huaian, Taizhou and detailed distribution of Salmonella samples from carcass swab-samples, environmental samples, equipment samples and intestinal samples of five sits in Huaian in China will be analyzed using software program and statistic method.

Results and Discussion

Figure 2 shows that 1,096 pork samples was analyzed for finding the prevalence of Salmonella, which was include 154 samples that were positive for Salmonella. (LI *et al*., 2014) In addition, there were 163 samples recovered from 154 Salmonella-positive samples. Among them, there were 45 isolated from Nanjing, 55 isolates from Yangzhou, 33 isolates from Huaian and 30 isolates from Taizhou. (LI *et al*., 2014)

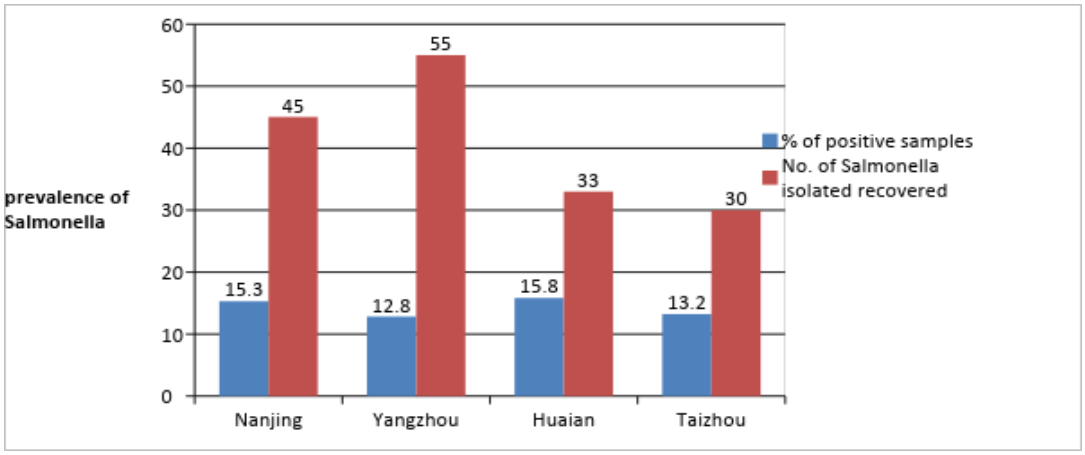

Figure 2: Prevalence of Salmonella in pork products from four cities in China

Figure 3 indicates that there were fourteen serovars which were identified from 163 Salmonella samples in four cities. (LI *et al*., 2014) From this it was clear that just Derby and Typhimurium existed in four cities and number of Derby was much higher than that of Typhimurium. Newport and Chester only existed in Nanjing, Virchow and Schwarzengrund only existed in Yangzhou, Agona only existed in Huaian and Limete just existed in Taizhou.

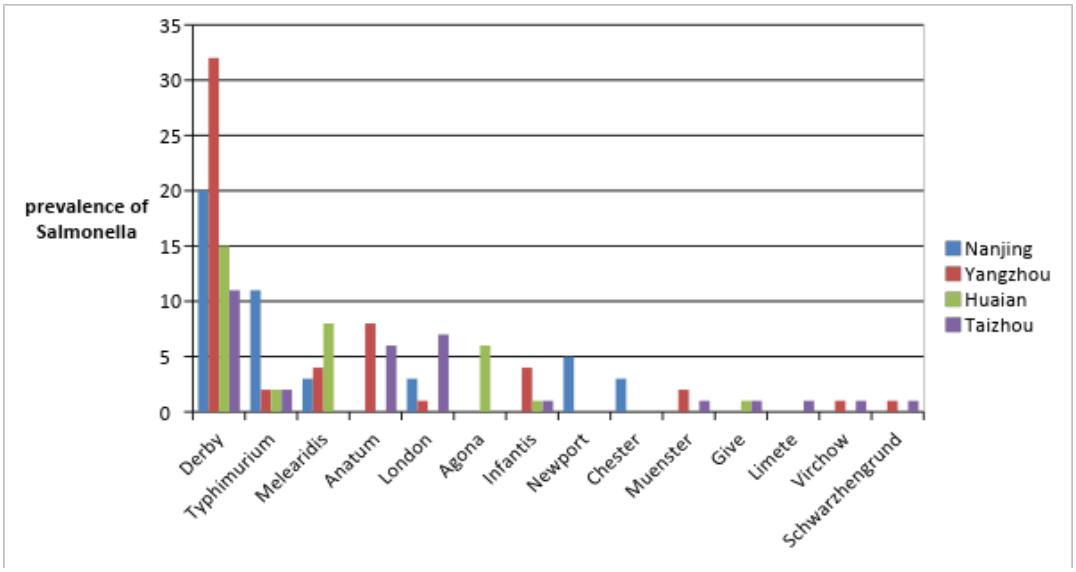

Figure 3: Serovar distribution of Salmonella isolates from four cities in China

Figure 4 (Zhou *et al*., 2017) shows the detailed distribution of Salmonella samples from carcass swab-sample, environmental samples, equipment samples and intestinal samples of five sites in Huaian in China. From this chart it was clear that carcass swab-sample was main source of Salmonella isolates.

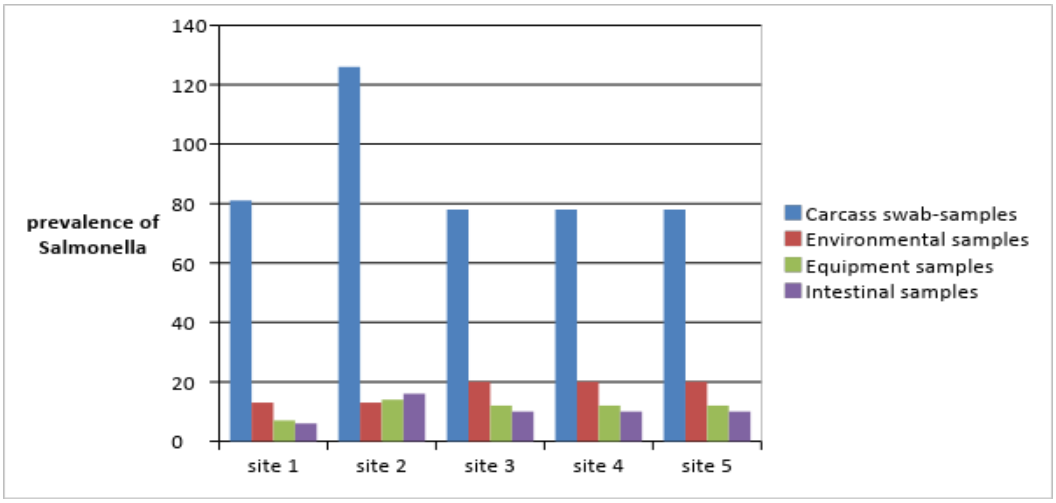

Figure 4: Prevalence of Salmonella isolated from carcass swab-samples, environmental samples, equipment samples and intestinal samples in Huaian in China

Conclusions

The aim is to find a useful model which predicts the occurrence of Salmonella in different sites and different processing from farm to fork. In QMRA, our research shows a high prevalence of Salmonella in the farm to fork chain of pork products and in processing areas.

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MICROBIAL ANALYSIS OF CRAFT AND MICROBREWED BEER

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Abstract

Unpasteurised and unfiltered craft and microbrewed beers and their microbial quality have been the focus of an increasing number of research papers in recent years due to a strong increase in their production and consumption worldwide. Commercially available Irish Red Ale craft beers were screened for a total viable count and the presence of lactic acid bacteria, *Enterobacteriaceae*, fungi and yeasts and heat-resistant bacteria. No *Enterobacteriaceae* or bacteria surviving the heat treatment were detected in any samples while the number of total viable bacteria ranged from an undetectable level to 2.7×10^3 CFU/ml and presumptive LAB were found in the range from an undetectable level to 3.8×10^3 CFU/ml. Yeasts were found in one sample. The overall low presence of bacteria in the analysed craft beers suggests the maintenance of strict hygienic conditions in most Irish microbreweries.

Introduction

Craft beers are usually produced in small breweries which differ from well established brands brewed by industrial large-scale breweries. Differences concern the taste and ingredients used but also the production process. As opposed to large-scale beer, craft beer is generally not pasteurised or sterile-filtered during the final production steps, rendering it more susceptible to microbial growth (Menz *et al.*, 2010; Giovenzana *et al.*, 2014; Garofalo *et al.*, 2015; Maifreni *et al.*, 2015). In addition, small breweries usually do not possess the same degree of quality control compared to large breweries with well-equipped laboratories and a large investment capacity (Giovenzana *et al.*, 2014). Also the operational management differs and brewing equipment in microbreweries with small annual production capacities may not be in use for a certain downtime during which resident microorganisms can reach high levels (Maifreni *et al.*, 2015).

Due to their increasing popularity, craft and microbrewed beer experienced a strong growth in many countries worldwide with Ireland accommodating 91 breweries in 2016 (BOE, 2017). However consumers may experience quality faults more frequently, as several studies on the microbial quality of craft beer suggest. Menz *et al.* (2010) detected lactic acid bacteria in almost 30% of craft beers tested and Giusto *et al.* (2005) found lactic acid bacteria in almost all samples analysed. Also Poveda *et al.* (2017) isolated lactic acid bacteria from 14 of 16 samples taken during a craft brewing production process. Various contaminants were further found by Garofalo *et al.* (2015) who examined the brewing environment, yeast pellets and spoiled products from a craft brewery. Of concern are also the findings of Jeon *et al.* (2015) who analysed several alcoholic beverages among which were draft, pasteurized and microbrewed beer and who found microbrewed beer to be contaminated the most. Apart from containing the highest number of bacteria, the study further found microbrewed beer to be contaminated with *Bacillus cereus* most frequently, with more than 50% of samples affected.

The objective of this study was to analyse craft beer samples for the presence of contaminating bacteria using culture-dependent methods.

Materials and Methods

Four Irish craft brewed Red Ale beer samples (table 1) were purchased and analysed in the laboratory for the presence of several groups of microorganisms: total viable count; lactic acid bacteria (LAB); *Enterobacteriaceae*; fungi and yeasts; heat-resistant bacteria. The beer samples were transferred into sterile bottles and flasks for subsequent analysis. For each of the media and conditions tested, 100µl of beer was plated in triplicate. Following incubation, bacterial colonies were counted and documented as CFU/ml.

Total viable count
100µl of beer was plated onto Plate Count Agar (Oxoid) and incubated aerobically at 37°C for up to 5 days.

Detection of lactic acid bacteria
For the detection of lactic acid bacteria, De Man, Rogosa and Sharpe agar (Oxoid) was used and the plates were incubated in triplicate at 30°C and 37°C aerobically and at 30°C under anaerobic conditions for 5 days.

Detection of Enterobacteriaceae
Screening for *Enterobacteriaceae* was undertaken on Violet Red Bile Glucose Agar (Oxoid) and aerobic incubation for up to 5 days at 37°C.

Detection of fungi and yeasts
The presence of fungi and yeasts was analysed with the help of Sabouraud Dextrose Agar which was prepared using Sabouraud Dextrose Broth (Oxoid) and Bacteriological Agar (VWR Chemicals). Aerobic incubation was undertaken for 5 days at 37°C.

Heat treatment for the detection of heat-resistant bacteria and spores
For the detection of heat-resistant bacteria and spores, samples of beer heat-treated for 15, 30 and 45 min at 80°C were spread plated onto Plate Count Agar (Oxoid). The plates were incubated aerobically at 37°C for up to 5 days.

Table 1. Information regarding the analysed beer samples

Sample number	Beer type	Information
Sample 1	Irish Red Ale	Bottled craft beer, unpasteurised, unfiltered, cleared through centrifugation step
Sample 2	Irish Red Ale	Bottled craft beer, unpasteurised, filtered
Sample 3	Irish Red Ale	Bottled craft beer, no information available on pasteurisation or filtration step
Sample 4	Irish Red Ale	Bottled craft beer, unpasteurised, unfiltered, bottle conditioned, contains yeast sediment, chilled distribution

Results and Discussion

Four Irish craft beer samples from different breweries were screened for the presence of contaminating microorganisms using non-selective and selective growth media. The results are shown in tables 2 and 3. Sample 1 contained lactic acid bacteria and the obtained colonies vary in number dependent on incubation conditions. The lowest number of 0.3×10^1 CFU/ml was obtained from plates incubated aerobically at 37°C while the highest number of 3.7×10^1 CFU/ml was detected on plates incubated

aerobically at 30°C. A further analysis involving bacterial identification will help to quantify the number of different species or strains detected, if more than one species is present, and to infer possible beer spoilage abilities. No *Enterobacteriaceae* or fungi and yeasts were detected in sample 1 and the total viable count yielded 0.7×10^1 CFU/ml. No cells survived the heat treatment procedure. In both samples 2 and 3 no colonies could be detected in any test performed. The low detection rate of bacterial colonies in the first three analysed beer samples suggests the maintenance of strict hygienic conditions and effective sanitation regimes in the breweries. Sample 4 which is a bottle conditioned beer, as shown in table 1, contains the highest number of bacteria. Lactic acid bacteria were detected in the range of 3.0 to 3.8×10^3 CFU/ml and the total viable count yielded slightly lower counts while no *Enterobacteriaceae* and heat-resistant bacteria were detected. The detection of microorganisms on SDA plates was expected due to the yeast sediment present. Further characterisation of the isolates will help to define whether the colonies grown on SDA belong to the desired brewing yeasts or whether contaminating wild yeast strains were present. The higher detection rate of contaminating bacteria in sample 4 may suggest a contamination of the pitching yeast culture or may originate from the brewing environment, for instance equipment. All analysed samples tested negative for the presence of bacteria or spores with the ability to survive the performed heat treatment.

Table 2. Results of the microbial analysis of craft beer

	Lactic acid bacteria			*Enterobacteriaceae*	Fungi and yeasts	Total viable count
Growth medium	MRS Agar	MRS Agar	MRS Agar	VRBGA	SDA	PCA
Incubation	30°C, 5d	37°C, 5d	30°C, 5d, anaerobic	37°C, 5d	37°C, 5d	37°C, 5d
Sample	Results in Colony Forming Units per ml (CFU/ml) (mean values of triplicate test)					
Sample 1	3.7×10^1	0.3×10^1	1.3×10^1	0	0	0.7×10^1
Sample 2	0	0	0	0	0	0
Sample 3	0	0	0	0	0	0
Sample 4	3.4×10^3	3.0×10^3	3.8×10^3	0	5.2×10^3	2.7×10^3

Table 3. Results of the heat treatment method

	Heat treatment at 80°C		
	15 min	30 min	45 min
Sample	Results in Colony Forming Units per ml (CFU/ml) (mean values of triplicate test)		
Sample 1	0	0	0
Sample 2	0	0	0
Sample 3	0	0	0
Sample 4	0	0	0

Conclusions

Microbial analysis of beers through culture-dependent methods on non-selective and selective growth media was used to determine the microbial quality of the beer and to evaluate the effectiveness of

sanitation regimes in the brewery which are especially important in the production of unpasteurised beers. The presence of either no bacterial colonies or low bacterial numbers in most of the analysed craft beer samples suggests a high microbial quality and the maintenance of effective sanitation regimes in the breweries. The results from this study do not suggest a difference in quality between large-scale and microbrewed beers, and further lead to the conclusion that a pasteurisation step is not necessarily required for a beer product free from contaminating bacteria. However, the microbial analysis of one craft beer sample yielded a higher bacterial count, suggesting a possible contamination of the pitching yeast culture or brewing equipment. Future work may involve the analysis of further craft beers whereby the emphasis is placed on breweries as small as possible with beers as unprocessed as possible. In addition, a preliminary identification and characterisation of the isolates might be conducted using for example biochemical tests in combination with 16S rRNA gene sequencing.

Acknowledgements

This study has been undertaken in the microbiological laboratory of the University College Dublin and resources required for the study have been provided by the college. The authors thank the college for making this study possible and further acknowledge the help and support of technicians and students working in the laboratory.

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Friedrich Westerholt, BE, M.EngSc.

Project Title: Surveillance of bacterial pathogens in dairy product facilities using molecular analysis.

Project Leader: Prof. Francis Butler

Abstract

Cronobacter spp. is an opportunistic pathogen widely associated with powdered infant formula (PIF). Because *Cronobacter* spp. can cause neonatal death, it is a pathogen of major concern for the PIF industry, and for the production of dairy ingredient powders that will be used in the production of PIF. In the past end product testing has been the main tool, in combination with the EU microbiological criteria (MC), to control the risk of *Cronobacte*r spp. being present in PIF. The objective of this study is to develop the use of product and environment surveillance, using molecular techniques, to identify contamination 'hot-spots', which are the source of the product contamination. This would allow the reduction of pathogen present in the final product, and allow for a prediction in relation to the concentration of *Cronobacter* spp. present in the final product. The study involved surveillance of a dairy ingredient plant over a thirteen-month period, with powder samples taken at twenty-minute intervals. The powder samples were tested for the presence of *Cronobacter* spp. using the ISO22964 (2017) method. Positive samples were confirmed using RT-PCR. The isolates identified as part of the sampling process underwent whole genome sequencing (WGS) allowing for a phylogenetic analysis to be undertaken. The results from the early part of the study allowed a more targeted follow up sampling to be conducted in another part of the production line. A Bayesian model was developed to quantify the concentration of *Cronobacter* spp. present in the dairy powder. The study showed a very high level of *Cronobacter* spp. present in the product, both in the wet and the dry production sections. The bioinformatic analysis of the sequence data allowed for the identification of two different sequence types (ST) throughout the study. The metadata showed that these two STs were persistent and clonal throughout the surveillance period. This allowed for the identification of a 'hotspot' that is likely the source of one of the STs. The follow up study confirmed this source to be identified. The study allowed for the development of a methodology for surveillance of PIF and dairy ingredient plants. A combination of plant surveillance, and end product testing, are an effective method for reducing the concentration of pathogens, and for identifying pathogen 'hotspots' throughout the production line.

Selected Recent Publications

von Westerholt, F., Gonzales-Barron, U., Butler, F. (2016) 'A Bayesian approach to estimating the uncertainty in the distribution of *Cronobacter* spp. in powdered infant formula arising from microbiological criteria test outcomes', *Microbial Risk Analysis*, 4, 36-42.

COMPARISON OF FRONT-FACE FLUORESCENCE SPECTROSCOPY AND FOURIER TRANSFORM INFRARED SPECTROSCOPY AS PROCESS ANALYTICAL TOOLS IN DAIRY INGREDIENT AND INFANT FORMULA MANUFACTURE

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Abstract

Front-face fluorescence spectroscopy (FFFS) and Fourier transform infrared spectroscopy (FTIR) were employed as process analytical technology tools to investigate the impact of heat treatment on skim milk powder, whey protein concentrate powder, demineralized whey powder and infant milk formula (IMF). This study investigated the use of FFFS at excitation wavelengths associated with tryptophan while a broad-spectrum approach was used with FTIR. This preliminary study demonstrated the potential of FFFS and FTIR for discrimination of dairy ingredient and monitoring the pre-heat process treatment and storage conditions of IMF.

Introduction

Dairy ingredients and infant milk formula (IMF) manufacturers constantly strive to improve the quality and the nutritional composition of their products. Standard IMF formulations are typically based on bovine skim milk solids mixed with whey protein, lactose, and vegetable oils in ratios representative of human milk (Murphy, Fenelon, Roos, & Hogan, 2014). A critical capability for milk processors is the ability to implement rapid, non-destructive and robust process analytical technology (PAT) systems which demonstrate control of, and confidence in, the specifications and properties of the powdered products required by the nutritional and infant formula industries. There is a need to develop and validate technologies such as fluorescence or IR spectroscopy which have the potential to be utilized as online PAT tools (Pei et al., 2011).

Fluorescence spectroscopy is a rapid and sensitive technique, which exploits the environmentally dependent properties of fluorescent compounds. Recently, fluorescence has been increasingly applied in food research in conjunction with new chemometric approaches to provide valuable information relating to product composition or structure. For example, fluorescence may be used to characterize changes at molecular level resulting from heat treatment (Lakowicz, 2007). Fluorescence spectroscopy has strong potential for use in dairy processing due to the presence of several intrinsic fluorophores, mainly the aromatic amino acids (tryptophan, tyrosine and phenylalanine), vitamin A and riboflavin (Hougaard, Lawaetz, & Ipsen, 2013).

The aim of the study was to carry out a preliminary investigation of front face fluorescence spectroscopy and Fourier transform infrared spectroscopy, combined with multivariate statistical analysis, as a PAT tool for discriminating between dairy ingredients and predicting pre-heat process treatment and storage conditions of IMF.

Fourier transform infrared spectroscopy (FTIR) spectroscopy measures the absorption of radiation by samples in the frequency range from about 4000-400 cm-1. The absorption involves transition between vibrational energy states and rotational substates of the molecule. A selection rule applies to these transitions and absorption of infrared light only occurs when the vibration causes a change in the dipole moment of the molecule. This makes it possible to find absorptions for specific functional groups; therefore, it can provide information about the secondary structure of proteins. FTIR spectroscopy in combination with attenuated total reflection (ATR) which requires little or no sample preparation is widely used for analyzing dairy products (Kamal & Karoui, 2015). Previous studies found that FTIR can be used to develop quantification models for nutritional parameters in commercial milk and non-solid fat content in milk (Bassbasi, Platikanov, Tauler, & Oussama, 2014).

Materials and methods

Rehydrated SMP, WPC, DWP and Model IMF were heat-treated (72, 95, 115 °C) at a flow rate of 2 L/min using a MicroThermics Lab heat exchanger (MicroThermics, NorthCarolina, U.S.A.) using a holding time of 15 s, evaporated and spray-dried using a pilot-scale spray dryer (Teagasc, Moorepark, Co. Cork, Ireland).. Each IMF batch was stored at 15 °C ± 2 °C and 37 °C ± 2 °C for one year and analysed at month 0, 3, 6 and 12.

Spectroscopic techniques

Fluorescence measurements were carried out using a Cary Eclipse fluorescence spectrofluorimeter and spectra of SMP, WPC, DWP and IMF were obtained using Cary eclipse software (Agilent Technologies, Little Island, Cork, Ireland). Scans were performed at 290 nm giving emission spectra of tryptophan (305 to 450 nm) (Schamberger & Labuza, 2006) in triplicate at room temperature.

FT-IR was used with attenuated total reflectance (ATR) to provide spectroscopic data on the physical state of IMF in triplicate Mid-infrared spectra were acquired using a single reflection diamond ATR instrument mounted in a nitrogen-purged Bruker Tensor 27 FT-IR spectrometer (Bruker Optik GmbH, Ettlingen, Germany), equipped with mercury cadmium telluride detector.

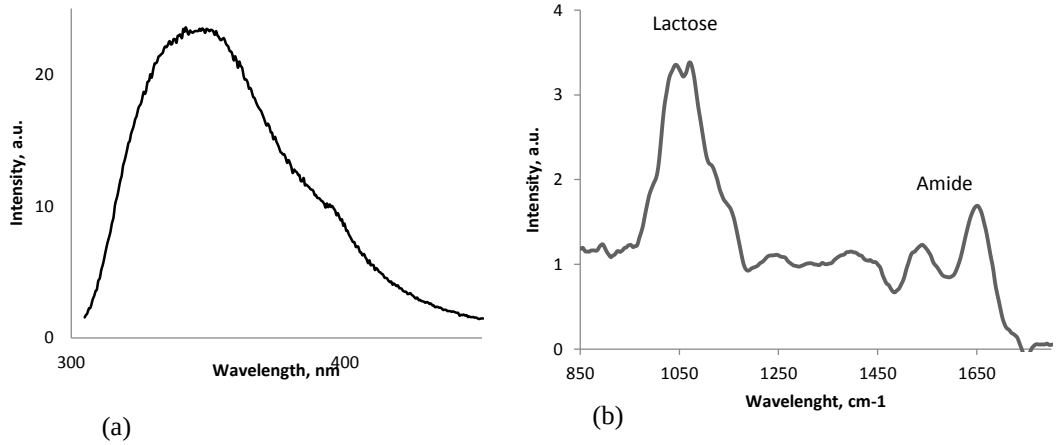
Multivariate analysis

Principal component analysis (PCA) and partial least squares (PLS) regression were performed using Unscrambler X 10.3 (CAMO, Norway). PCA was applied, as an initial step to illustrate discrimination of batches by grouping according to variance. PLS regression model performances were evaluated on the basis of the magnitude of the R2 (correlation coefficient of determination) and root mean square errors in cross validation (RMSECV) (Woodcock, Downey, & O'Donnell, 2009).

Results

Dairy ingredient discrimination by PLS-DA using FFFS and FTIR.

FFFS and FTIR were used for the discrimination of 36 batches of dairy ingredients (SMP, WPC and DWP). Typical spectra obtained from an SMP batch is shown in Figure 1. Principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) were performed to discriminate between dairy products. The spectral data for dairy ingredient discrimination pre-treatment consisted of detrending and SNV prior to modelling. The most effective discriminative models were tryptophan group frequencies for FFFS and amide and lactose bands for FTIR. Perfect classification was achieved for SMP, WPC and DWP (100% accuracy, specificity and sensitivity). These results demonstrate the potential of FFFS and FTIR for discriminating between dairy ingredients.



(a) (b)

Figure 1: Representative FFFS emission spectra of tryptophan for SMP and FTIR amide and lactose bands for SMP in powder state (b).

Prediction of pre-process and storage temperature and storage time.

Front face fluorescence

The Martens' uncertainty test (Martens & Martens, 2000) was applied to improve the performance of PLS models developed using FFFS spectra. Table 2 shows the number of variables selected to build the models using 84 samples. When no improvement was achieved in using the uncertainty test, all 284 variables were used to build the models. Storage temperature was predicted with an RMSECV value < 2.7 °C. The FFFS models predicted storage time with an RMSECV value of 1.5 months. However, these models were further improved when segregated by storage conditions as shown in Table 2. Models predicted pre-heat process temperature with an RMSECV value of 6.7 °C. Reduced RMSECV values of 4.2 °C and 4.1 °C for 15 °C & 37 °C storage were achieved for models developed using samples segregated by storage temperature

Table 2: PLS models for model IMF using FFFS Tryptophan excitation 290 nm, emission 305-450 nm

	FFFS	Sample	Factors	RMSECV	R2	Variables
Storage temperature (°C)	15°C & 37°C	84	9	2.7	0.941	134
Storage time	15°C & 37°C	84	8	1.5	0.881	133
(month)	15 °C	48	7	1.2	0.952	120
	37 °C	48	7	1.0	0.954	170
Pre-heat process	15°C & 37°C	84	7	6.7	0.855	142
temperature	15 °C	48	8	4.2	0.945	181
(°C)	37 °C	48	7	4.1	0.956	141

Fourier transform infrared spectroscopy

FTIR spectral data was pre-treated with detrending and SNV prior to mean centering. FTIR models developed for storage temperature successfully differentiated (R^2 = 0.710 and RMSECV < 5.9 C) between 15 °C & 37 °C storage samples (Table 3). Storage time was predicted with an RMSECV of 1.3 month and R^2 value of 0.909, model performance was further improved by segregating samples by

storage temperature to RMSECV values of 1.1 and 0.9 month for 15 °C & 37 °C storage respectively. Prediction of pre-heat process temperature was unsuccessful using FTIR spectra.

Table 3: PLS models for model IMF using FTIR; 1200-850 cm-1

	FTIR	Samples	Factors	RMSECV	R^2	Variables
Storage temperature (°C)	15°C & 37°C	84	7	5.9	0.710	11
Storage time	15°C & 37°C	84	7	1.3	0.909	73
(month)	15 °C	48	5	1.1	0.940	50
	37 °C	48	6	0.9	0.961	49
Pre-heat process	15°C & 37°C	84	1	17.6	0.000	208
temperature	15 °C	48	1	17.5	0.000	208
(°C)	37 °C	48	20	14.5	0.463	208

Conclusion

FFFS and FTIR, coupled with multivariate data analysis, were found suitable for potential application as PAT tools in dairy ingredient and infant formula powder production. FFFS successfully predicted storage temperature, storage time and pre-heat process temperature. FTIR successfully predicted storage temperature time and storage time but was unsuccessful for pre-heat process temperature. Therefore, while both spectroscopic techniques have the potential to be used as PAT tools in the dairy ingredients and IMF industries, the results of the present study suggest that FFFS is the more versatile technology.

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Eithne O'Flaherty BSc, MSc.

Project Title: A risk assessment model examining the human exposure to antibiotic resistant bacteria through surface water ecosystems

Project Leader: Assoc. Prof. Enda Cummins

Abstract

Antibiotic resistant bacteria (ARB) are posing a serious threat to human health due to the complications in treating these types of infections. ARB are bacteria that were once killed by an antibiotic but can now resist the effects of that antibiotic. The overall objective of this project is to examine the human exposure to antibiotic resistant *Escherichia coli* (AR *E. coli*) through drinking, irrigation and recreational water. An extensive scientific literature search was carried out to collate data to model each step of the three probabilistic models. Microsoft excel 2013 with the @ risk add on was used to create each of the models. Monte Carlo Simulation was performed and probability distributions were used to characterise uncertainty and variability in the model input data to generate the output distributions. Sensitivity analysis using Spearman's rank order correlation was performed to examine the effect of the input data on the final human exposure results. Results from the drinking water model show the mean human exposure to AR *E. coli* from tap water consumption ranged between 2.47×10^{-8} and 2.09×10^{-2} cfu/100ml. The level of AR *E. coli* required in the source water to exceed the Drinking Water Directive (Council Directive 98/83/EC, 0 CFU/100 ml of *E. coli* in drinking water) varied between 1 and 5 log cfu/ml, depending on the water treatments used. The results from the irrigation model show the mean human exposure levels to AR *E. coli* through the consumption of irrigated lettuce was between 1×10^{-4} and 3×10^{4} cfu/g as a result of the different scenarios investigated. The results from the recreational model show the mean human exposure levels to AR *E. coli* ranged between 0 and 2 log per exposure event. The results generated by the drinking water model could be used to help set acceptable levels of AR *E. coli* in source water supplies. The irrigation model highlights the most suitable post-harvest treatments to use to reduce the human exposure to AR *E. coli* and also helps to set local guidelines for producers on maximum permissible contamination levels in irrigation water. The recreational model provides information on the possible human exposure levels to AR *E. coli* through recreational water use. The research done by this project is contributing to the current gap in the literature with regards to human exposure to ARB through environmental sources.

Recent Publications

O'Flaherty E and Cummins E. (2017). Antibiotic resistance in surface water ecosystems: presence in the aquatic environment, prevention strategies and risk assessment. *Human and Ecological Risk Assessment,* 23(2), 299–322.

O'Flaherty E., Borrego C. M., Balcázar J. L., and Cummins E. (2018) Human exposure assessment to antibiotic-resistant *Escherichia coli* through drinking water. *Science of the Total Environment,* 616-617, 1356-1364.

Kevin Hunt

Project Title: A Risk Assessment of Norovirus in Irish Produced Oysters

Project Leader: Prof. Francis Butler

Abstract

Contaminated food causes almost a third of infectious disease globally. Norovirus is the most common source of foodborne infection and causes more disease burden than any other pathogen. As a human-targeting virus, Norovirus enters the food chain through human effluent coming into contact with food. This can happen in three broad ways: irrigation of vegetables with contaminated water, unhygienic handling of food by food workers, and accumulation in the digestive glands of shellfish through shellfish filtration. Because of its unique transmission vector, and because oysters are typically eaten raw or lightly cooked, the risk posed to consumers by Norovirus in oysters requires a specific risk management approach.

The objective of this work is to assemble a quantitative probabilistic risk assessment framework for estimating the single-serving risk posed by Norovirus to consumers of Irish oysters. The study follows the standard Risk Assessment paradigm of Hazard Identification, Exposure Assessment, Hazard Characterisation (or Dose-Response), and Risk Characterisation.

The challenges in estimating exposure to Norovirus in oysters are that the virus is concentrated in the digestive glands, and that oysters are eaten by the individual unit, not by overall weight. A stochastic model linking number of oysters eaten and the distribution of virus copies within individual oysters is required. The first part of this project was to use real time RT-PCR to measure the amount of norovirus in individual oysters taken from the same harvesting area, in order to fit an appropriate distribution. This was repeated six times, half of which were treated post-harvest by purification. The second part took this new distribution, and used it to create a probabilistic exposure assessment for a single-serving meal. The third part is a survey of the most likely dose-response models available in the literature, which were then integrated into a full risk characterization estimate. This could then be used to estimate the risks associated with different scenarios of contamination and to assess the most important inputs to the overall risk, as well as the effectiveness of different intervention strategies for risk management.

Conference Presentations

Hunt K, Doré B, Keaveney S, Butler F. (2017) Estimation of illness arising from consumption of raw oysters exposed to water-borne norovirus. *Poster presented at: ICPMF10, the 10th International Conference on Predictive Modelling in Food*; 26-29 Sep 2017; Cordoba, Spain.

Hunt K, Doré B, Keaveney S, Rupnik A, Butler F. (2017) A quantitative method for estimating the likely intake of norovirus copies through consumption of Irish oysters. *ICMSS 2017, the 12th International Conference on Molluscan and Shellfish Safety*, 14-18 May 2017, Galway, Ireland.

Pat Doyle, BSc Dairying, BAgrSc, MAgrSc, MBA

Project Title: Risk ranking of bacterial pathogens in raw milk

Project Leader: Prof. Francis Butler

Abstract

The consumption of raw milk, which can have bacterial pathogens present, is a human health hazard capable of causing serious disease. The objective of this work was to develop a quantitative graphical risk ranking framework for bacterial pathogens present in raw milk produced in Ireland. Risk is generally considered a combination of the severity of the food hazard and the likelihood of its occurrence. Based on these two elements, severity and likelihood of its occurrence, a risk ranking approach using a graphical two-dimensional risk ranking grid is commonly used for risk ranking. There has been much interest in developing risk ranking criteria for hazards that are more quantitative and remove the potential confusion and subjectivity associated with such a simple risk ranking type approach. In the current work, the framework for risk ranking of bacterial pathogens in raw milk was based on a graphical two-dimensional risk ranking grid where the axes represent a measure of the severity of the pathogen and the likelihood of its occurrence. The severity of the pathogen was classified according to EC Directive 2000/54/EC (EC, 2000) which divides biological agents into four risk groups according to their level of risk of infection. The likelihood of occurrence of a bacterial pathogen in raw milk is potentially difficult to quantify. In Ireland and elsewhere, the data that is available is occurrence (presence/absence) data for bacterial pathogens present in bulk tank milk at farm level. A structured approach was adopted to firstly identify the potential bacterial pathogens present in Irish produced raw milk and this was followed by a systematic review of the literature to identify the occurrence of bacterial pathogens in farm bulk milk produced in Ireland. A detailed literature search identified fourteen bacterial pathogens potentially associated with Irish raw milk. However, Irish data for only seven of the pathogens was found following a systematic review of the literature. No one pathogen emerged as a 'highly risk ranked' pathogen. Rather, all seven pathogens have a sufficiently high likelihood of occurrence that results in a significant risk associated with the consumption of raw milk. Occurrence data for the rest of the EU indicated that there was not a major difference in risk from the consumption of raw milk between Ireland compared to the rest of the EU.

DETERMINATION OF LIPID CONTENT OF FRESH AND FROZEN-THAWED SALMON FILLETS USING HYPERSPECTRAL IMAGE TEXTURE AND SPECTRAL FEATURES

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Abstract

This experiment is carried out to research the lipid content on fresh and frozen-thawed salmon fillets by applying short-wave near infrared (400-1000nm) hyperspectral imaging system. Hyperspectral cubes will be captured, and their corresponding spectra data will be analysed. Principal component analysis (PCA) is applied to explore the variance between two conditions of salmon. Partial least squares- discriminant analysis (PLS-DA) lipid content on fresh and frozen-thawed salmon fillets will be used to build classification models for recognition and authentication of the tested samples. The study will offer an analysis model for testing lipid content of salmon fillets. The results will indicate that hyperspectral imaging could be used to determine lipid content on fresh and frozen-thawed salmon fillets.

Introduction

Hyperspectral imaging is a rapid, non-destructive and reagent-less analytical technique employed widely in diverse fields including agriculture (Monteiro *et al*., 2007) and food (Gowen *et al*., 2009; Barbin *et al*., 2012). Hyperspectral imaging combines aspects of conventional imaging and spectroscopy providing both spatial and spectral information of a sample (Gowen *et al*., 2009). The information is gathered in two spatial dimensions and a spectral dimension in the form of a hypercube. Each pixel of the image contains an entire spectrum, thus hyperspectral images are rich in information. Hyperspectral imaging in the near infrared region is a possible method of predicting quality parameters of biomass pellets.
Salmon are rich in unsaturated fatty acid and unique texture and flavour. Lipid content is one of most important compound of quality, flavour and nutrients. Given the perishable nature of fish, extension of its shelf life is necessary, and freezing is an excellent and commonly used way (Zhu *et al*., 2013). However, during freezing, storage, and thawing, fish muscles go through a progressive deterioration in nutritive value, texture, and other functional properties (Karoui *et al*., 2006). It is therefore important to have rapid, reliable methods of lipid measurement.

There are some approaches for assessing the lipid content of fish: chemical analysis, the Torry fat meter, computerized tomography (CT) and near-infra-red (NIR) spectrophotometry and calibration (Fjellanger *et al*., 2000).Recent advances in the area of computers and image processing have created new ways to monitor quality in the food industry (Brosnan and Sun, 2004). Stien *et al*., (2007) set up a rapid and automatic measurement of lipid content in salmon fillets by utilizing computer vision system and found that lipid content could be assessed based on image analysis. However, when comes to the comparison between fresh and frozen-thawed salmon in terms of lipid content, there isn't a proper measurement and a sophisticated model to assess it. Therefore, it is urgent to build a model to assess the lipid content prediction at two conditions, which is the major factor for fish quality. Therefore, **the main objective of this study is to investigate the lipid content of salmon fish by a near infrared hyperspectral imaging(HSI) system for collecting lipid pixels in fresh and frozen-thawed salmon filets.**

Materials and Methods

Fish sample preparation
Sixty Atlantic salmon (Salmon salar) fillets originated from a farm in Ireland were labelled and then transported to laboratories of Food Refrigeration and Computerized Food Technology (FRCFT), University College Dublin (UCD), Ireland. Each fish fillets will be about 200g and full length varied from 27.5 to 32 cm (average 30.5 cm). Upon arrival, samples were randomly divided into 2 groups with equal numbers: fresh (Group 1), chill-stored (Group 2) at -18 °C refer to the samples subject to storage for 7 days at controlled refrigerated condition.

Chemical Analysis
When fresh and F-T samples reach 10°C, it will be sent to HIS. After the collection of hyperspectral images, samples will be immediately tested, and fat contents will be measured by Soxhlet extraction method using petroleum ether (AOAC 2006). Each analysis will be performed in duplicate. Samples will be immediately put in individual plastic bags and placed in an insulation box to maintain the constant temperature of 8-12 °C after image collection.

Hyperspectral imaging system
Spectral images of the salmon fillet stored for different days will be acquired in reflectance mode by using a laboratory-based pushbroom hyperspectral imaging system. The system is made up of a camera with a C-mount lens (Xeva 992, Xenics Infrared Solutions, Leuven, Belgium), a spectrograph (ImSpector, N17E, Spectral Imaging Ltd, Oulu, Finland) with a near infrared wavelength from 900 to 1700 nm, two tungsten illuminating lamps (Vlight, Lowel Light Inc., New York, USA) positioned at an angle of 45° to light up the translation stage, which was operated by a stepping motor (GPL-DZTSA-1000-X, Zolix Instrument Co. Beijing, China), and a computer system consisting of imaging data acquisition software (Spectral Cube, Spectral Imaging Ltd., Oulu, Finland). The wavelength interval is 3.34 nm between contiguous bands and produce 256 bands in total.

Hyperspectral image acquisition and calibration
Each salmon fillet is firstly placed on the translation stage and then conveyed to the field of view (FOV) of the camera to be scanned line by line. After eliminating noisy signal at the beginning and end of the spectral region, 180 wavebands are retained for each spectrum.

Data analysis
Matlab R2015a software (The Mathworks Inc., USA) will be used for image processing. Prior to data analysis, Savitsky Golay smoothing and derivatives (SG) and standard normal variate (SNV) will be used as spectral pretreatment to remove the undesired effects in sample measurements, such as random measurement noise, interfering consequences of unwanted chemical and physical variations. Then principal components analysis (PCA) exploration is applied for spectral analysis.

Chemical imaging
Chemical imaging is the technique for creating visual color images to show the quantitative spatial distribution of components in heterogeneous food products. The model is then applied to predict component concentration at each pixel in hyperspectral images of the 30 prediction samples, leading to the production of chemical images.

Expected results and Discussion

Statistics of Measured Reference Values
Literature review : The descriptive statistics such as minimum, maximum, mean, and standard deviation (SD) for reference fat values measured were summarized in Table 1. (Zhu, *et al*,2013)

Table 1. Summary of chemical analyses for fat (based on wet weight) and moisture in calibration and prediction samples

Components	Calibration				prediction			
	Min	Max	Mean	SD	Min	Max	Mean	SD
Fat (%)	3.30	25.13	10.41	4.97	4.44	12.78	8.21	2.49
Moisture(%)	54.89	74.73	67.58	4.26	65.24	72.22	69.13	2.10

Expected results: In my study, chemical analyses of fat for fresh and F-T salmon will be compared with the prediction samples, like what literature review shows. High correlation line of fat content between fresh and F-T salmon will close to r = 1.

Overview of the Spectra

Literature review: The NIR absorbance (log 1/R) spectra from 20 samples of each whole fillet were averaged (Fig. 1). The absorptions of fat and moisture in NIR spectral range are the theoretical basis for establishing the mathematical correlation between spectral data and compositional contents. (Zhu *et al*.,2013)

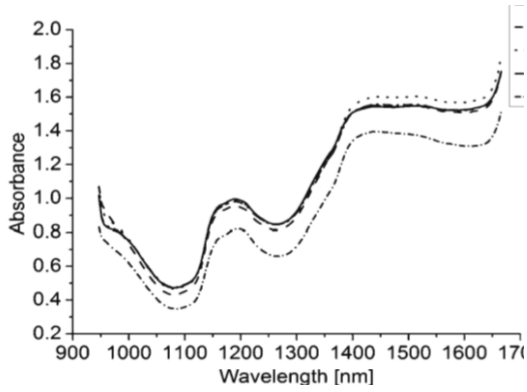

Fig 1. Averaged NIR absorbance(log1/R) spectral of 20 samples of each whole fillet

Expected results: In my study, the NIR spectral image will be argued. The trend of curve will be compared in terms of lipid content. The curve of fresh salmon should be higher than F-T salmon.

PLS Models

Literature review:The performances of PLS regression models use reflectance spectra for fat between fresh and frozen-thawed. Different spectral transformations are also tested in modeling, showing that reflectance, absorbance. In addition, t values of 1.82 and 1.41 for fat and moisture were obtained, respectively. The two-sided t critical value at 5 % significance level for 19 degrees of freedom was 2.09, suggesting no significant difference between predicted and reference values for both models. The above accurate results confirmed the suitability of hyperspectral imaging for fat and moisture prediction in salmon. (Zhu *et al*.,2013)

Table 2. Results of PLS regression models for fat and moisture in salmon fillets

components	calibration		Cross-validation		prediction			
	Rc	RMSEC (%	Rcv	RMSECV (%)	Rp	RMSEP (%)	t	t(19, 0.05)
Fat	0.96	1.21	0.95	1.40	0.93	1.24	1.82	2.09
Moisture	0.97	0.86	0.95	1.10	0.94	1.06	1.41	2.09

Expected results: t value and t(19,0.05) will be discussed. The predictive model and chemical analysis will be compared by this two value. If they are in the acceptable range, the model will be confirmed the suitability of hyperspectral imaging for fat in salmon.

Chemical Images for Fat

Literature review: The chemical images of fat and moisture for the 20 prediction samples are shown in Fig. 5 (sample positions refer to Fig. 1). The changes in fat and moisture contents were assigned with linear colour scales. Different colours represented different concentrations of the predicted chemical compositions. Pixels having similar spectral patterns in original hyperspectral images would produce similar predicted values of fat or moisture, and then would appear in similar colours in the resulting chemical images. (Zhu *et al*.,2013)

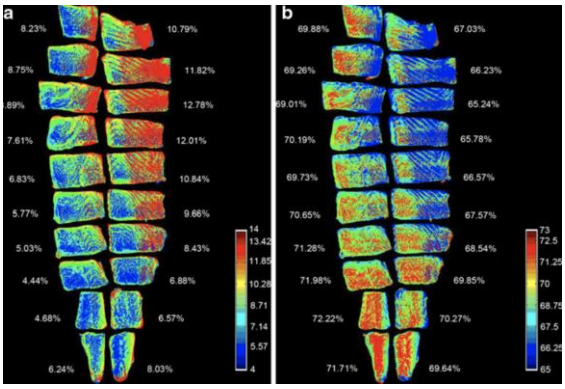

Figure 2. Chemical images of fat (a) and moisture (b) for the 20 samples in prediction set

Expected results:the chemical map of fat distribution will be showed in different color. The area of fat content in fresh salmon will be larger than the F-T salmon.

Conclusions

This study will demonstrate the great potential of hyperspectral imaging for determination of lipid content between fresh and frozen-thawed salmon. The successful outcome of this study would be very advantageous for company to characterize the good quality fish.

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DETECTION OF FOOD BORNE BACTERIA ON CULTURE MEDIA BY NIR HYPERSPECTRAL IMAGING

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Abstract

For sustainable food production and effective control of foodborne illnesses, rapid detection of bacteria in food is essential. The present work is a preliminary study for identification of foodborne bacteria by NIR Hyperspectral imaging. Two strains of *Bacillus* and one strain of *Chronobacter* were grown on nutrient agar up to six decimal dilutions using spread-plate technique. Samples were imaged with NIR (880-1720nm) pushbroom hyperspectral system. Spectral profiles for each strain were compared through Principal Components Analysis (PCA). Partial Least Squares Discriminant Analysis (PLS-DA) for each spectral range was calibrated on the highest microbial concentration and applied to subsequent dilutions to predict microbial strain. The results demonstrated 89% of correct pixel classification for dilution 10^{-1} between the three bacteria, while model application to further dilutions presented poor results (65% to 0.3%), illustrating the need for improvement of model robustness. This approach was investigated to provide the knowledge base for a robust and early-stage identification of food borne bacteria.

Introduction

Food safety and compliance to legislation are of utmost importance to the food industry as it pertains not only to licensing of a company, but also the health of the consumers. It is for this reason, that development of rapid, accurate and objective quality inspection systems throughout the food process is important (Wu and Sun, 2013). Culturing and colony counting takes several days to detect bacteria owing to long incubation periods and identification requires further biochemical tests to be conducted. Advanced methods such as ELISA (Enzyme Linked Immunosorbent Assay) and PCR (Polymerase Chain Reaction) highly reduce the analysis time. However, these methods require trained personnel and continuous purchase of expensive antibodies and reagent kits (Eady *et al.,* 2015).Thus the conventional culture techniques, immunological methods and PCR are unsuitable for detection of spoilage and pathogenic bacteria in large quantities of food products manufactured day in and out (Feng and Sun, 2014).

NIR Hyperspectral imaging combines NIR spectroscopy and computer vision to obtain both spatial and spectral data in one system (Feng and Sun, 2014). Hypercubes (Hyperspectral images) are three-dimensional blocks of data composed of two spatial and one wavelength dimension. The hypercube allows observation of various constituents of a sample, separated into specific regions of the image, since regions with similar spectra tend to have similar chemical composition (Gowen *et al.,* 2010). Chemometrics includes different pre-treatment methods and modeling tools, used to analyze the spectra. In most image analyses, spectra extracted from hyperspectral images are generally pre-treated to enhance signal quality. The pre-treated spectra are then correlated with measured true values using tools like PLS-DA (Feng and Sun 2014).
The objective of the study was detection and discrimination of bacteria on agar using NIR Hyperspectral imaging.

Materials and Methods

Sample preparation

Following bacterial isolates were evaluated: *Bacillus amyloliquefaciens*, *Bacillus subtilis*, and *Chronobacter sakazakii*. Each bacterium was streaked on sterile Nutrient agar Petri plates (Disposable Sarstedt Petri Dish, 92mm x 16mm) for obtaining isolated colonies. The petri plates were incubated at 37^{o} Celsius for 24 hours. The colonies so obtained were picked up using a sterile loop and immersed in 4.5 ml Ringers solution to form the zero dilution. The culture from zero dilution was further diluted up to 10^{-6} using Ringers solution. Ten-fold dilution scheme was used for carrying out the dilutions. All the dilutions were plated in duplicates on sterile Nutrient agar Petri plates using spread plate technique. The Petri plates were incubated at 37^{o} Celsius for 24 hours. Nutrient agar was chosen because it is a general growth medium containing only peptone, beef extract, sodium chloride and bacteriological agar. Ringers solution was used as an isotonic diluting fluid for suspending the bacterial cells. It is isotonic with bacteria and thus prevents them from being subjected to osmotic stress when they are removed from their habitual environment. All procedures were performed under aseptic conditions. After incubation, the plates were allowed to equilibrate with the ambient temperature for about 30 minutes before imaging.

NIR Hyperspectral imaging

A pushbroom NIR (880–1720 nm) hyperspectral imaging system (DV Optics, Padova, Italy), was used to acquire the images of Petri plates. Raw images were collected in radiance and converted into reflectance format using white and dark reference scans. A 100 % reflectance standard tile was used as a white reference. The plastic lids of petri plates were replaced with glass lids (Lime soda glass) in class II Laminar air flow hood in order to avoid the NIR signals from plastic lids. Thereafter, images of the entire Petri dish, without removing the lid, were collected. One image per bacterial species and dilution was collected (18 images in total).

Data analysis

For white correction, reflectance images were obtained by dividing raw by the average spectra of a white reference tile (using SScanner software). Further data analysis was performed in Matlab (Version R2017a, Mathworks, USA). The spectral range at the edges of the hyperspectral system detection range were discarded. Wavelength range retained was from 978nm to 1643nm. Black table and tile background were masked using a threshold obtained by applying Otsu method (implemented with the function "graythresh" in Matlab) at wavelengths 1083 nm and 1643nm, respectively. The effect of the plastic edges at the border of the petri dishes was removed by morphological operations in the image, by eroding the masked petri dishes in the image by a circular structuring element of 25-pixel diameter. For pre-processing, spectral range was limited between 978nm and 1363 nm. These cleaned images for the three microbes were concatenated for each dilution to form mosaics. PCA was performed for individual images with two PCs (Principle Components), gathering 98 % of the variance. PLS-DA models were calculated for each group. Evaluation of the model performance was done by determining the proportion of correctly classified pixels (CC); proportion of pixels correctly assigned to Gram positive and Gram negative groups (CCGram); and proportion of pixels of *Bacillus* samples correctly classified as the right *Bacillus* species (CCB).

Results and Discussion

Culture growth

Post incubation, matt growth was obtained from dilution 10^{-1} till the dilution 10^{-4}, clustered growth was obtained at dilution 10^{-5} and few isolated colonies were obtained with clustered growth at the dilution 10^{-6} (Figure 1) for all the three bacterial isolates.

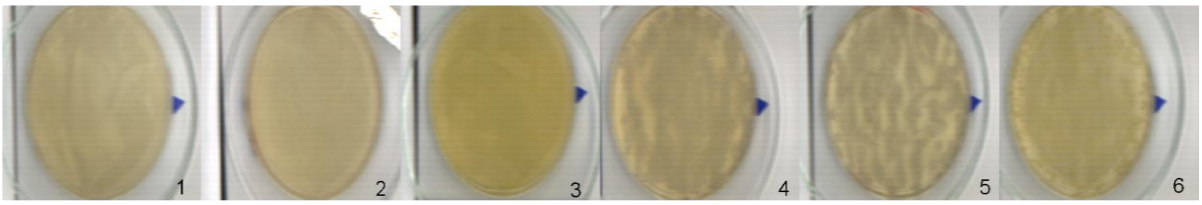

Figure 1. Dilution 10^{-1} for (1) *B.amyloliquefaciens* (2) *B.subtilis* and (3) *C.sakazakii* and dilution 10^{-6} for (4) *B.amyloliquefaciens* (5) *B.subtilis* and (6) *C.sakazakii*

Exploratory analysis and classification Results

PCA scores on the first and second principal components (98% of the variance) showed a differentiation between Gram positive and Gram negative bacteria (Figure 2) in dilution 1(10^{-1}) samples (Figure 1), PCA scores for the two species of Bacillus (Gram positive) overlapped in a greater measure (results not shown).

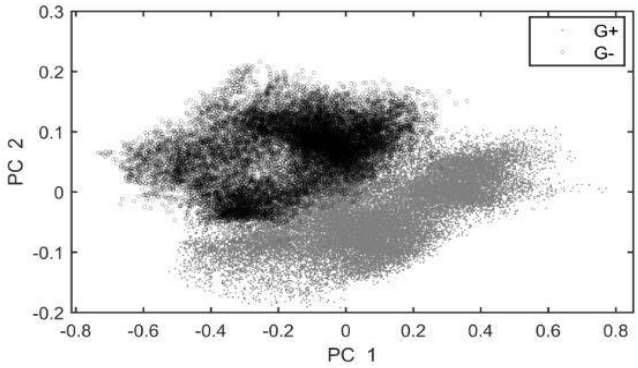

Figure 2. PCA scores on PC1 and PC2. Gram category for each point is identified in the legend.

Regarding the PLS-DA (Table 1), good classification results (CCGram=0.99; CC=0.89) were obtained on the calibration image (Dilution 10^{-1}, as shown in Figure 3). When applying the model to further dilutions, correctly classified pixels (CC) between the three species of bacteria ranged between 0.50 to 0.18. From dilution 10^{-2} to dilution 10^{-6}, the model was able to distinguish between Gram negative and Gram-positive bacteria with a range of CC pixels 0.18 to 0.65 and between different species of *Bacillus* with a range of CC pixels between 0.01 to 0.22.

Validation	CC	CCGram	CCB
Dilution 1	0.89	0.99	0.55
Dilution 2	0.18	0.18	0.01
Dilution 3	0.50	0.65	0.17
Dilution 4	0.34	0.36	0.0033
Dilution 5	0.35	0.55	0.015
Dilution 6	0.36	0.61	0.22

Table 1. *PLS-DA result:* Proportion of correct classified pixels (CC) for each Dilution and classification modality.

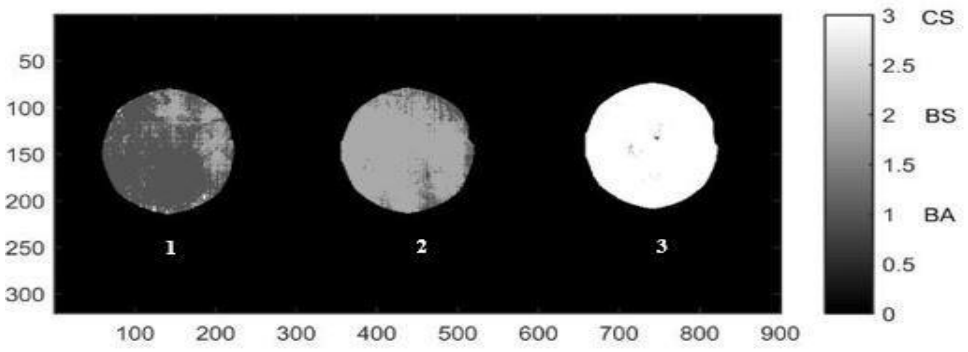

Figure 3. Prediction map of PLS-DA model for Dilution 10^{-1}, colormap scale indicates the bacteria species (1:*B.amyliliquefaciens*, 2:*B.subtilis*, 3:*C.sakazakii*).

Conclusions

Three foodborne bacteria, *Bacillus amyloliquefaciens*, *Bacillus subtilis* and *Chronobacter sakazakii*, grown on culture media, were characterized and classified in this work through hyperspectral imaging. Exploratory analysis (PCA) allowed characterization of spectral differences between bacteria, particularly between gram-positive and gram-negative species. A multivariate classification model (PLS-DA) allowed to successfully identify the three species of bacteria on the same samples used for calibration, while poor classification results were obtained when applying the model to lower dilutions. Future work will aim at improving the robustness of the model by including data from several replicates and dilutions in the calibration and considering lower dilutions for model validation. This study is part of wider multimodal approach, carried out to provide robust and early-stage identification of food borne bacteria through hyperspectral imaging.

Acknowledgments

Funding for this research was provided by Science Foundation Ireland (SFI) under the investigators programme Proposal ID 15/IA/2984—HyperMicroMacro.

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DEVELOPMENT OF CHEMOMETRIC MODELS TO PREDICT WATER ACTIVITY OF WHEAT FLOUR

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Abstract

This project investigates the effect of different storage conditions of the wheat flour using NIR spectroscopy. The spectral data obtained from NIR spectroscopy were pre-processed using chemometrics. Wheat flour samples were prepared with different water activity values using refrigeration, thermal treatments and various storage conditions. Chemometrics analyses including Principal Component Analysis (PCA) and Partial least squares (PLS) modelling were used to predict moisture content in wheat flour samples. The results of PLS prediction performance revealed R^2C of 0.99 and R^2CV of 0.90 with RMSECV of 0.03 A_w for wheat flour.

Introduction

Wheat flour is widely used food ingredient .Water activity is one of the important factors affect the quality of powder spray drying or heat processes and storage (Yang *et al.,* 2016). Wheat flour is a primary ingredient for the some of the world foodstuffs such as cereals, cake, biscuit, noodles, bread and pasta. Water activity affects wheat flour properties during different heat treatment processes (Samuel *et al.,* 2016). Near-infrared (Vis/NIR) spectroscopy is a valuable technique for rapid, non-destructive, and online analysis of the quality and composition of agricultural products (Aernouts *et al*., 2011).

The objective of this study was to develop chemometrics models for the prediction of water activity of wheat conditions using NIR spectroscopy.

Materials and Methods

Sample preparation
Whole wheat flour powder was purchased from a local store in Ireland. 18 replica of each powder were prepared. The initial water activity of powders were measured using Aqualab Model series 3(Decagon Device, Inc. Pullman, Washington) water activity instrument. The weights of the samples were also measured. Six replicas of both milk powder and wheat flour were subjected to an ambient condition for 2-3days. Other six of each powder were kept in an oven (45℃) and a refrigerator (4°C) for 3 hours before the NIR measurements.

Vis-NIR Spectroscopy
Vis-NIR spectra were collected using a NIR Systems 6500 instrument (NIR Systems. Inc., Maryland, USA). A ring cup (7.5 cm diameter and 1.5 cm-height) incorporating an optical window of a diameter of 5.5 cm was filled with the powder sample and sealed with a backing lid. Reflectance spectra log (1/R) were acquired and recorded over the spectral range 400 - 2498 nm with 2 nm intervals. Samples were scanned in duplicate in random order at room temperature (~ 20 ^oC).

Chemometric analysis

In this study spectral data in csv format were imported to Unscrambler software (v9.7; Camo, Trondheim, Norway).The spectral range of wavelength of 957nm-1657nm are obtained for wheat flour subjected to different atmospheric condition were analysed. Principal component analysis (PCA) was performed to identify sample clusters of different water activity. Partial least squares (PLS) regression was carried out for the prediction of water activity in samples. The performance of PLS regression models was assessed using root mean square error of cross-validation (RMSECV) and regression coefficient of determination based on cross-validation (R^2CV).

Results and Discussion

NIR spectra

In the initial experiment three replicas of fresh wheat flour, wheat flour kept at room temperature and the sample kept in the refrigerator and there NIR spectra are shown in Figure 1. All the three spectra have very similar spectral shape; while the spectrum of a Fresh powder shows higher amplitude of log (1/R) than the other two spectra. This difference occurs due to the exposure of the replica to different storage conditions. It was found that water activities of wheat flour samples kept in a refrigerator are higher than that of samples kept at room temperature.

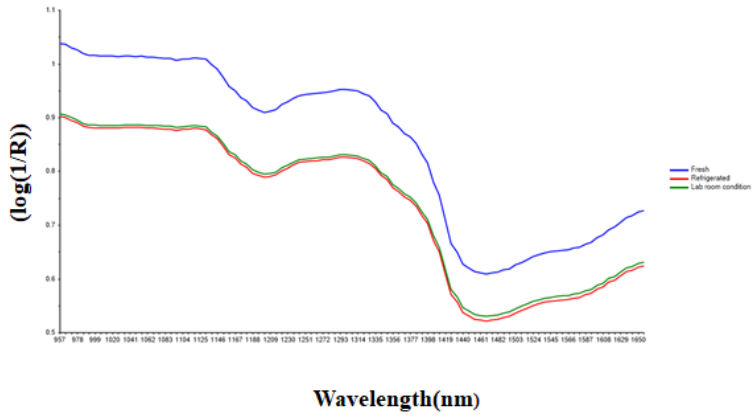

Figure 1. NIR spectra Log (1\R) of wheat flour

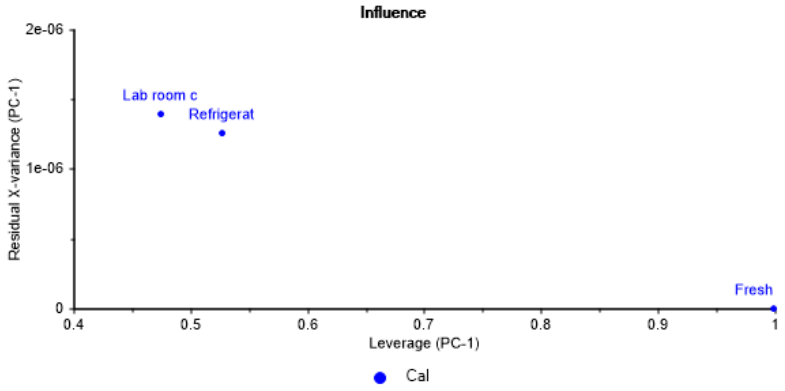

Figure 2. A scattered plot of Principal component analysis for wheat flour

Figure 2 shows the scatter plot of PCA based on the spectral data of wheat flour kept in three different atmospheric conditions. It shows that the two samples kept in a refrigerator and room temperature are located close to each other but likely exist in a different cluster from the location of the fresh sample.

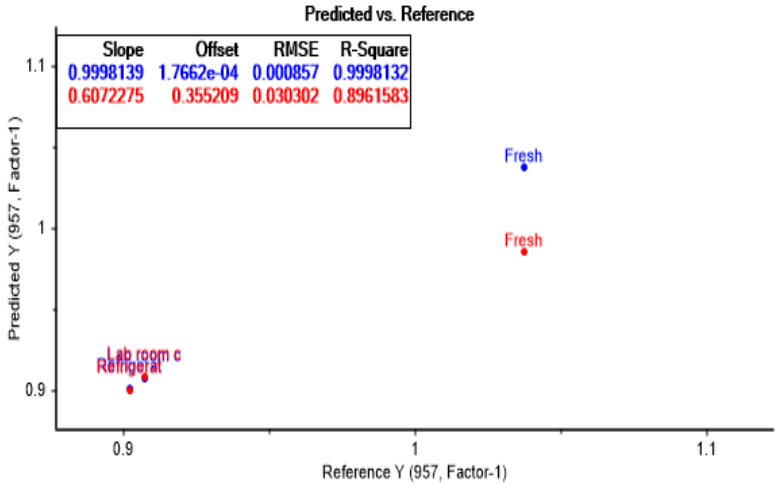

Figure 3. Partial least square regression of wheat flour

In Figure 3, the PLS model plot (predicted water activity values vs. reference values) for the three conditioned samples. Model performance revealed R^2C of 0.99 and R^2CV of 0.90 with RMSECV of 0.03 Aw (water activity).

Conclusions

Results demonstrated that the storage temperature had major effects on the water activity (Aw) of the wheat flour. PCA analysis and PLS modelling show the differences between the samples. However, limited samples were used in the current study.. In a future study, the experiment will be conducted using more wheat flour samples designed with different water activity levels to approve the potential of NIR spectroscopy for the quality control of wheat flour.

Acknowledgements

The authors wish to thank for technical supports from Dr. Ming Zhao, Dr. Anna Lesniak Podsiadlo, Dr Ana Herrero Langreo, Mr Xiao Wang and Miss Eva Achata.

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DISCRIMINATION OF ORGANIC WHEAT FLOUR FROM OTHER FLOUR VARIETIES BY NEAR-INFRARED (NIR) HYPERSPECTRAL IMAGING

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Abstract

Wheat is a vital food crop for human activities and daily life which supply about half of the people on earth. This paper takes organic wheat flour (cassava flour, ordinary wheat flour, organic Spelt flour) as the research object and uses the near-infrared spectroscopy technology and hyperspectral technology with the advantages of rapid and non-destructive testing to test the system which includes two types flour by measuring effective chemometrics methods. A variety of chemometric methods have been used to screen flour adulteration system and to obtain a more suitable measurement model.

Introduction

HIS (hyperspectral imaging), which is a new technology that combines the knowledge of spectroscopy and machine vision acquires spectral and spatial information from one object at the same time (Dale *et al*., 2013). Due to the abundance of information, hyperspectral imaging widely uses for nondestructive analysis of agricultural and food production. Properties of hyperspectral imaging are that both the spatial information and the spectral information of the detected object can be obtained at the same time (Magwaza *et al*., 2011). Therefore, this technology can detect the external quality of an object and detect the internal quality and the safety of an object like a spectroscopic technique.

Food safety is becoming an urgent challenge in this world. Activities such as cultivation, culture, processing, packaging, storage, transportation, sales and consumption of food must comply with international and national standards (Fulponi, 2006). Food safety covers: production and operational safety; outcome and process safety; real and future safety. Although there are many ingredients in the flour, the necessary ingredients of the nutritional quality and processing quality of the flour are water, protein, starch, wet gluten, dry gluten, and gluten index. The gluten content is related to protein content and gluten index reflects the protein quality (Day *et al*., 2006).

Near-infrared spectroscopy has used in the analysis of food composition for more than 30 years, and the relevant analytical research reports have published for decades (Pasquini, 2003). AACC (American Association for Clinical Chemistry) has 10 to 15 topics each year related to food research. The advantage of Near Infrared Spectroscopy is that it can determine the various components in the food and measure the number of parameters related to the idealised properties of the food simultaneously. The application of near-infrared spectroscopy in food detection is becoming more and more common, for example, the analysis of starch in wheat shows its water solubility, and the determination of protein content can determine its hardness. Also, the determination of moisture changes in starch structure reflects the degree of saccharogenic.

The objective of this study was to distinguish the organic wheat flour from other flour varieties by near-infrared (NIR) hyperspectral imaging.

Materials and MethodsMaterials and Methods

Adulteration production

The materials in this study are 4 adulteration types (a, b, c, d): a. Organic wheat flour(OWF) (variety: Avatar, origin: Ireland) and corn flour (CoF); b. Organic wheat flour(OWF) and cassava flour (CaF); c. Organic wheat flour (OWF) and plain wheat flour (WF);d. Organic wheat flour (OWF) and organic Spelt flour (OWF). The Organic wheat flour (origin: Ireland) samples were certified by the Organic Trust Ireland (IE- ORG-03, EU/non-EU Agriculture), whose chemical composition was: 75.3% of carbohydrate, 10.1% of proteins, 1.4% of fat, and 3.1% of fibre. Within each set of sample types, 1-40 samples of Calibration set are pure OWFs, and 41-140 samples are corresponding impure samples; 1-20 samples of Prediction set are pure OWF, and 21-70 are corresponding impure samples.

Data analysis

Hyperspectral imaging requires calibration to account for the spectral and spatial variation of the light source, detector response, and system optics (Gaufrès *et al*., 2017). To obtain a reflectance hyperspectral image, the original hyperspectral image should be calibrated with a black and white reference image. Since the amount of data in hyperspectral images is usually tremendous and there is a problem of collinearity, which needs stoichiometric algorithms to dig out detailed and vital information. MATLAB is a multi-functional computational language and interactive environment development algorithm that creates models analyses data visualises images. Analyzes hyperspectral image data by using Matlab make this process effectively.

Based on the experimental data and use of Matlab software to master a variety of spectral pretreatment methods. Then, using PLDA, SVM, etc. to establish a full-wavelength discriminant model and analysis the comparative of the model based on different pretreatment methods.

Calibration models in this study will be established by correlating the image profiles and the reference values with a chemometric method, such as partial least squares (PLS) regression, artificial neural network (ANN) as well as support vector machine (SVM), etc. After the full wavelength models, simplified models can also be developed by several essential wavelengths for calibration. Various variable selection methods are available, including VIP score, PLS regression coefficients method, genetic algorithms, stepwise regression, successive projection algorithm. The established model should be validated by either cross-validation or external validation (predicting unknown samples). During the processes of calibration and validation, coefficients of determination for calibration (r^2C) and validation (r^2V) and RMSE of calibration (RMSEC) and cross-validation (RMSECV) are to be used for evaluating the performance of the calibrated model. Generally, a good model should have high values of r^2C and r^2V, low values of RMSEC and RMSECV, and a small difference between RMSEC and RMSECV.

Results and Discussion

Expected results

Perez-Mendoza et al., (2003) propose near-infrared spectroscopy combined with partial least squares method for the non-destructive and rapid detection of flour quality. Thirty flour samples containing talcum powder are prepared, and the near-infrared diffuse reflectance collects the range of 12500 to 4000 cm-1 of the product. After collecting, selecting the optimal spectral pretreatment method and spectral range, using partial least squares (PLS) to establish a quantitative analysis model. The results show that the correlation performance of the established quantitative analysis model is high relatively; also the prediction correlation coefficient and the prediction root mean squared error are meet the requirements. It can be acknowledged that

near-infrared spectroscopy is feasible for the rapid non-destructive detection of adulteration of flour.

In the research of Guo et al. (2018), the SVM model established by the radial basis function was used to discriminate the true and false egg powder in the qualitative discrimination. The results showed that the three types of egg powder (whole egg powder, egg yolk powder, and egg white powder) had correct identification rate of adulteration whose rate is more than 90 present. It shows that the combination of hyperspectral technology and chemometrics model can identify pure egg powder and adulterated egg powder effectively. In quantitative detection, the relationship between spectral data and adulterated content was established by using a partial least-squares regression model, and the performance was reasonable by using this model.

Su and Sun (2016) develop a new method of wavelength selection and proposes a multispectral real-time imaging system for the staple food industry to identify three adulterants which includes rye flour (RF), organic wheat flour (OWF) and spelt flour (SF). First, a calibration model was established by partial least squares discriminant analysis (PLSDA) and partial least-squares regression (PLSR).

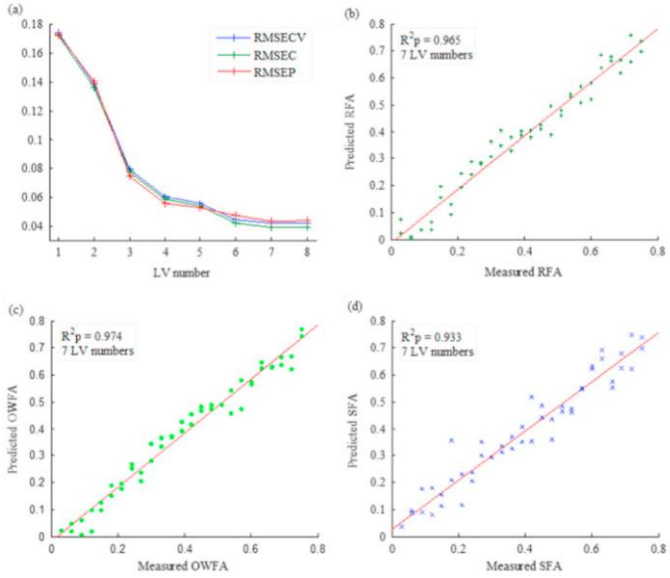

Figure 1 (a) Selection of the latent variable (LV) numbers in PLSR model; measured and predicted values of (b) RFA, (c) OWFA, and (d) SFA in OSF estimated by PLSR model for the validation set using the selected characteristic wavelengths (Su and Sun, 2016).

Spectral preprocessing was used for multivariate analysis of hyperspectral images in the 900-1700 nm spectral range. In the simplified PLS-DA and PLSR models, there is better performance of OSF qualitative identification and pseudo-component quantitative measurement. The average cross-validation coefficient (r^2CV) was 0.958, and the predicted value (r^2P) was 0.957. The results show that spectral imaging combined with multivariate analysis can quickly assess the purity of organic spelt flours.

From the perspective of near-infrared hyperspectral technology development, the selection of algorithms and the update of spectral technologies have brought about rapid development in this field. At present, the application of near-infrared hyperspectral technology in flour adulteration has a vast space because of the development of computer algorithms. The purpose of this study is to provide a more appropriate and efficient inspection system.

Based on the experimental data and full wavelength model, applying the second derivative, regression coefficient (RC) of PLSR, GA, SPA and other methods to establish different feature-wavelength models. Then compare and analyse the advantages of models based on

different feature wavelength selection methods. This method can optimise the innovation feature wavelength selection methods.

Conclusions

The most critical challenge for this study is to design a new wavelength selection method for real-time determination of three types of dopants in OSF using hyperspectral imaging. These completed studies have provided broad prospects and predictable results for this experiment. The overall goal of the project is to apply hyperspectral imaging to determine the main distinguishing substances and use them as a tool for flour production monitoring.

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EFFECT OF SONICATION ON THE RHEOLOGICAL AND OPTICAL PROPERTIES OF PECTIN

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Abstract

This study investigated the effect of sonication on the rheological and optical properties of pectin dispersion. A 2% (w/v) pectin dispersion was sonicated at different pulsation cycles for 5 minutes at 25^{o}C. The sonication frequency for all the treated samples was kept constant at 20 kHz. Sonication affected the rheological and optical properties of pectin dispersions. It was found that the viscosity and absorbance values for the sonicated samples were lower compared to the thermally treated samples. The low absorbance values elucidated the reduction of polymeric junction zones for the sonicated samples. The results demonstrated the shorter pulsation cycle was directly proportional to absorbance and viscosity of the samples.

Introduction

Pectin is a water soluble polysaccharide with high molecular weight. Commercially, pectin is extracted by acidification, followed by alcoholic precipitation from apple pomace or citrus peel. Pectin dispersions are widely used in food industries as gelling, stabilizing or thickening agents. They are used in preparation of jams, jellies, desserts, soft drinks, dairy products and also pharmaceuticals (May 1990; Wang *et al.,* 2016).

Ultrasound processing also know as sonication is a widely used processing technique in the food industry. Its application includes the production of stable emulsions, extraction, pasteurization, sterilization and meat tenderization (Seshadri *et al.,* 2003; Chemat *et al.,* 2011). Ultrasonic waves are high-frequency sound waves ranging between 20 kHz to 200 MHz having ability to produce mechanical, thermal and chemical effects also known as intense local effect due to phenomenon known as cavitation. Cavitation includes growth and collapse of micro-bubbles which leads to generation of high temperatures and pressure within a liquid during its sonication (Tiwari *et al.,* 2010; Chatel 2017).

Studies shown that ultrasound can be used for synthetic polymeric solutions containing long chains for controlled degradation resulting reduction of their molecular weight (Price 1990; Pingret *et al.,* 2013). Various authors have suggested that cavitation is the main phenomenon responsible for degradation of these polymeric chains (Mason *et al.,* 1992; Crum 1995; Mason and Cordemans 1996; Stephanis *et al.,* 1997). Pectin dispersion upon sonication demonstrates reduction in viscosity and turbidity. More transparent dispersion gels can be formed as the sonication time period is increased (Seshadri *et al.,* 2003).

The objective of this study was to evaluate the effects of sonication on the rheological and optical properties of pectin dispersion.

Materials and Methods

Sample Preparation – Hydrocolloid

Pectin powder from apples (Sigma-Aldrich Ireland Ltd, Dublin, Ireland) was used for the sample preparation. Pectin dispersion of 2% (w/v) was prepared by adding 2g of pectin powder into 100 ml of deionized water. The dispersion was mixed continuously with the help of a magnetic stirrer at 20^{o}C for 30 minutes. The thermal treatment involved heating the pectin

dispersion at 100^{o}C for 5 minutes. The evaporated water was re-added to maintain the concentration of the samples.

High-Intensity Ultrasonication

1,500 W ultrasonic processor (VC 1500, Sonics and Materials, Inc., Newtown, USA) with 19 mm probe was used for sonication treatment. All sonication treatments were performed at constant frequency of 20 kHz and 50% amplitude level for 5 minutes. The first treatment involved pulse duration of 5 s on and 5 s off and the second treatment was continuous without any pulse duration. The amplitude level for both treatment was kept at 60%.

Rheological Measurements
Samples viscosity was analyzed using Brookfield digital viscometer (Model DV – II+ Version 2.0). P-12 spindle was immersed into 50 ml of pectin sample for the viscosity measurements. The value of viscosity was recorded from the viscometer display which appears in units of centipoise (cP) or milliPascal-seconds (mPa.s).

UV-Visible Absorption Spectroscopy
The absorbance value for pectin dispersions was analysed using UV-3100 PC Spectrophotometer. 3 ml of pectin solution was placed in quartz cuvette (QC 521) and absorbance was recorded in 230-480 nm region.

Results and Discussion

Effect of Sonication on Rheological Properties of Pectin Dispersions – Viscosity

The viscosity of the sonicated and thermally treated pectin dispersions is given below in Fig 1. It was found that as the pulsation cycle time was reduced, the dispersion became thinner showing reduction in viscosity. Additional energy was transmitted into the pectin dispersion due to reduction in pulsation cycle. This ultimately led to increased cavitation effect which aided in breaks down of polymeric chain of the pectin resulting in decreased viscosity.

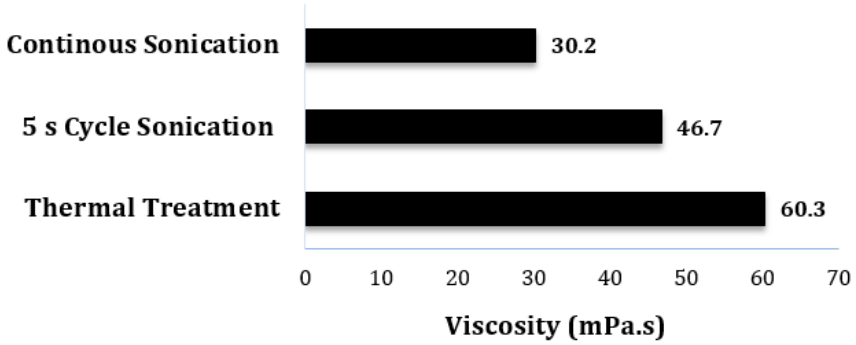

Figure 1: Effect of sonication and thermal treatment on viscosity of pectin dispersion.

Effect of Sonication on Optical Properties of Pectin Dispersions – Absorbance

It was found that high-intensity sonication altered the optical properties of the samples. The sonicated sample were significantly less turbid as indicated by their low absorbance value in table 1 measured at 280 nm. The lower absorbance values for sonicated samples signify a reduction in polymeric chain length due to enhanced energy dissipation into the sample. Fig. 2 illustrates the absorbance spectra of UV- visible light (Range: 230 – 480 nm) for different treatment conditions of pectin dispersion. The scattering of light depends upon the formation of discrete junction zones in dispersion (Tang *et al.*, 2001). Thermally treated sample forms a strong network consisting series of junction zones. In the sonicated samples, there was

breakdown of junction zones due to reduction in particle size of the sample. This resulted in reduced absorbance and scattering of light. Thus the sonicated samples were less turbid demonstrating more transparent dispersion.

Table 1: Absorbance of sonicated and thermally treated pectin dispersion at 280 nm.

Sample number	Treatment	Absorbance at 280 nm
1	Thermal treatment	1.68
2	5s cycle Sonication	1.46
3	Continuous Sonication	1.43

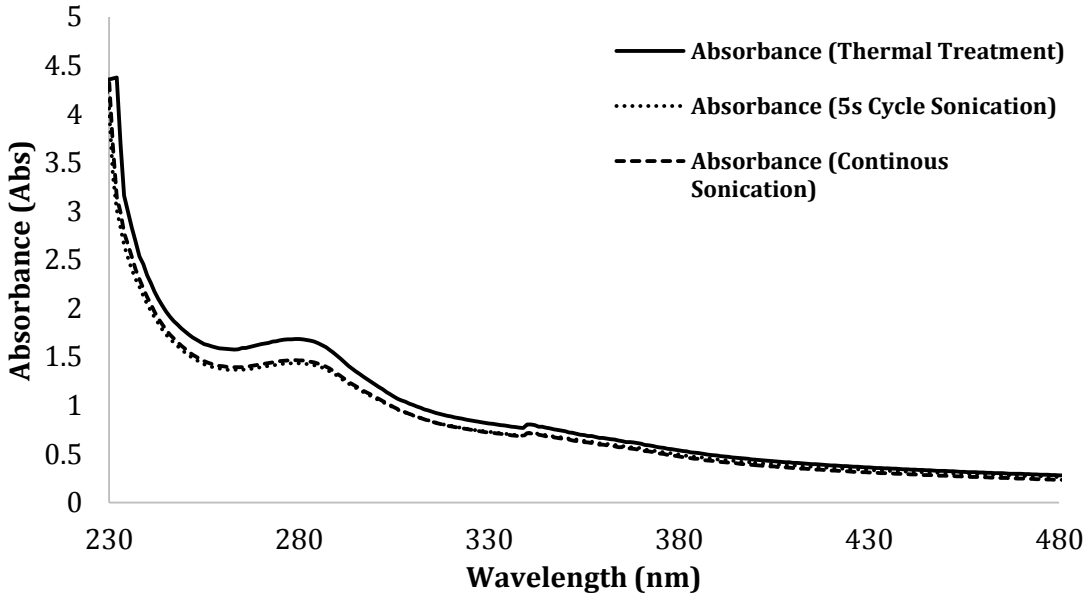

Figure 2. Absorbance spectra of sonicated and thermally treated pectin dispersion.

Conclusions

This study demonstrated that when the pulsation time is reduced, the viscosity and absorbance of pectin dispersion was also reduced. The rheological properties of sonicated samples were found to have a negative impact on the viscosity. However, the optical properties of the pectin dispersion can be improved through application of sonication. Sonicated samples from this study were found to be less turbid. Therefore, sonication could be beneficial for food industries involved in production of clear beverage and transparent jams or jellies.

Sonication can be potentially used by food industries to replace thermal processing. Such processing techniques can be employed to alter the flow properties of hydrocolloids such as pectin. Jellies made from citrus fruit like oranges contains thermal liable nutrition like vitamin C. Such heat liable nutrients can be preserved with the help of sonication which is a non-thermal treatment. Further investigation is required to evaluate the synergic effect of pulsation cycle and treatment time on the rheological and optical properties of pectin dispersion.

Acknowledgements

The authors acknowledge Dr. Anna Lesniak (Technical officer at UCD School of Biosystems & Food Engineering) for her continuous support during the research project.

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PREDICTION OF GEL STRENGTH AND CUTTING TIME DURING ENZYME INDUCED MILK COAGULATION USING NIR SPECTROSCOPY

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Abstract

Quality can be built into a food product by controlling the manufacturing processes through real time analysis of critical quality parameters. Real time estimation of milk gel firming and cutting time is essential for cheese making as it impacts cheese yield and quality. Near Infrared (NIR) light backscatter technology has proven successful in monitoring milk coagulation kinetics. A fibre optic sensor with near infrared light of 880 nm can determine the gel strength and predict the cutting time of milk gel. Thus, NIR spectroscopy can be effectively used as an in-line process analytical tool for the automation of the cheese plants. This study aims to predict the gel strength and determine the cutting time of enzyme induced coagulated milk using a fibre optic sensor at a range of process conditions.

Key words

Enzyme induced; Gel strength; Light backscatter; Near Infrared

Introduction

Coagulation of milk is a crucial step and a critical control point in cheese manufacture. It is induced by enzymatic action by addition of Rennet and terminated by cutting the formed milk gel to induce syneresis. Cutting the milk curd at low gel strength will decrease the cheese yield due to increased loss of fat and curd fines in the whey (Castillo *et al.,* 2000). Cutting too firm gel will retard syneresis resulting in high moisture cheese with undesirable properties (Castillo *et al.,* 2000). A decrease in moisture content even by 1% would cause reduction in yield and ultimately decrease in profits (Fagan *et al.,* 2008). Also, inadequate curd moisture content will have a negative effect on cheese ripening, its quality and price (Fagan *et al.,* 2008). Thus, it is pivotal to cut the milk gel at the right time in cheese plants.

Traditionally, the curd is cut after a predetermined time has elapsed from the enzyme addition or upon the operator's judgement based on empirical evaluation of firmness, evaluation of textural properties and visual appearance of the gel properties (Castillo *et al.,* 2000; Abdelgawad *et al.,* 2014). Also, variations in milk properties and processing conditions affect curd firmness and gel microstructure which will modify the optimum cutting time (Abdelgawad *et al.,* 2014). Thus, development of a monitoring and control technology for process automation is essential.

Several devices have been developed for monitoring milk coagulation and gel firming in the past decades by studying the rheological properties of milk gel. But these systems are destructive and cannot be applied for in-line application. An inline optical sensor was proposed by Payne *et al.,* in 1993 to monitor physicochemical changes in milk coagulation based on changes in light backscatter of near infrared (NIR) light. The light backscatter depends on milk composition, casein micelle and fat globule size (Abdelgawad *et al.,* 2014). Adaptability of optical spectroscopy to study variation in product formulation, processing conditions and study the factors influencing milk coagulation are being studied.

The objective of this study is to predict the gel strength and determine the cutting time of enzyme induced coagulated milk using NIR spectroscopy.

Materials and Methods

Experimental design
This experiment is designed to predict the cutting time of milk gel and study the effect of different temperatures, enzyme concentration levels and pH on the milk coagulation kinetics. Different experimental factors will be selected to obtain the diffuse reflectance profiles to achieve the objectives of this study. The milk coagulation process will be monitored using NIR light backscatter obtained from the CoAguLite sensor, small amplitude oscillatory rheometry (SAOR) as a reference method and clotting time will be visually determined.

Materials and Testing procedure
Commercial pasteurised milk will be used for this study. Rennet enzyme (CHY-MAX Plus 200 IMCU/ml) will be used to coagulate the milk.

A laboratory cheese-making vat fitted with fibre optic CoAguLite sensor will be used in which milk will be heated to a selected temperature level of 32^{o}C and the pH will be recorded. Rennet will be added to the heated milk and agitated for 3 mins. Similarly, this procedure will be repeated for different temperature levels, pH and enzyme concentration. 20 ml of this milk will be added to the sample holder of the rheometer.

Determination of NIR backscatter parameters
Reflectance measurements will be recorded simultaneously with enzyme addition to the milk. The CoAgulite sensor that will be used in this study consists of one 600 µm diameter fibre for light emission into the milk and one 600 µm diameter fibre for transmitting backscattered light from the milk to the photodetector (Fagan *et al.,* 2007). The optical data will be collected every 6 seconds from the fibre optic sensor with NIR light of 880 nm. The light backscatter profile will be calculated using linear-least square regression according to the procedure described by Castillo *et al.,* (2000). The light backscatter Ratio (R), first derivative ($R^{'}$) and second derivative ($R^{''}$) of light scatter ratio will be derived and the optical parameters will be defined as described in Table 1 (Abdelgawad *et al.,* 2014).

Table 1. Optical parameters derived from the light backscatter ratio profile

Parameter	**Units**	**Definition**
t_{max}	min	Time to the first maximum of $R^{'}$
t_{max2}	min	Time to the second maximum of $R^{'}$
t_{2max}	min	Time to the first maximum of $R^{''}$
t_{2min}	min	Time to the first minimum of $R^{''}$
t_{2max2}	min	Time to the second maximum of $R^{''}$
t_{2min2}	min	Time to the second minimum of $R^{''}$
$R^{'}_{max}$	min^{-1}	Value of $R^{'}$ at t_{max}
$R^{''}_{max}$	min^{-2}	Value of $R^{''}$ at t_{max}

Determination of Rheological and visual parameters
The rheological data will be collected every 25 seconds from the small amplitude oscillatory rheometry. Gelation time (t_{gel}) will be determined as the time when the gel reaches a storage modulus ($G^{'}$) greater than or equal to 1 Pa and cutting time (t_{cut}) will be determined as the time when the gel reaches $G^{'}$ = 20 Pa. Visual inspection will be done by inserting a spatula into the gel until there is an appearance of small flocks of casein on the surface of the spatula (Arango *et al.,* 2015).

Expected results and discussion

Previous experiments conducted to study milk coagulation kinetics and effect of different processing parameters on cutting time prediction using NIR spectroscopy give an idea about the expected results.

Clotting time, cutting time and t_{max} decrease as enzyme concentration and temperature increases and as pH decreases. Light backscattering in milk depends on the number and size of casein and fat particles and wavelength of incident radiation. The light backscatter ratio increases with increasing particle size of casein network.

Cutting time can be predicted by an algorithm proposed by *Payne et al.*, (1993): $t_{cut} = \beta\, t_{max,}$ where β is a regression coefficient and a function of temperature, enzyme concentration and pH. Figure 1 shows the typical results obtained from NIR light backscatter readings during rennet induced milk coagulation process.

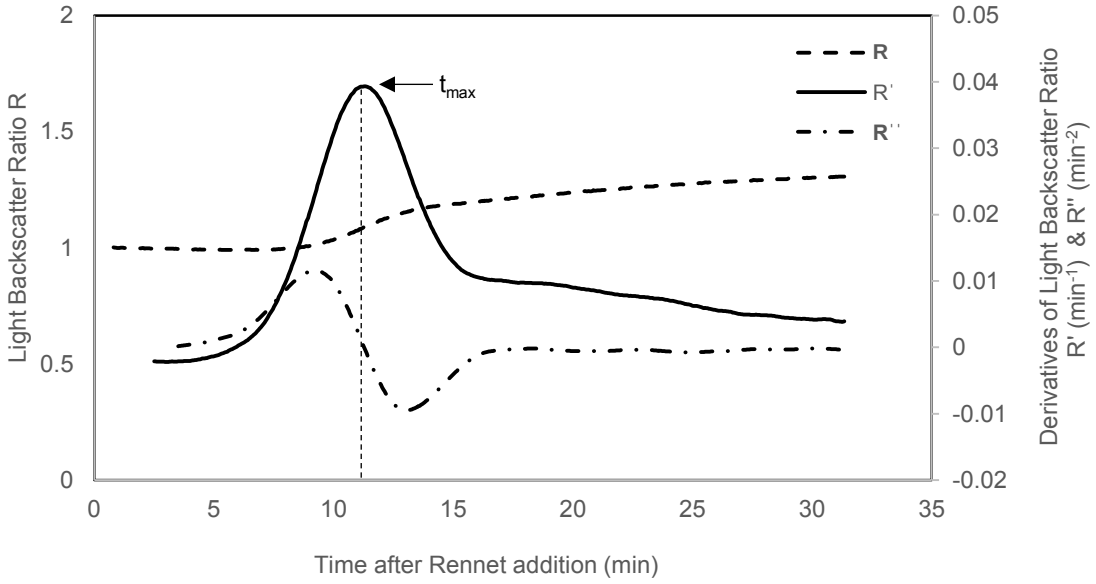

Figure 1. Light backscatter profile and its derivatives as a function of time

The optical parameter t_{max} is strongly correlated to the rheological parameter $t_{G'20}$ as seen in Figure 2. This confirms that cutting time can be predicted by determining time to the first maximum of the first derivative of reflectance ratio (R). This time-based parameter generated from the diffuse reflectance profile is a function of coagulation rate which varies with temperature, enzyme concentration and pH.

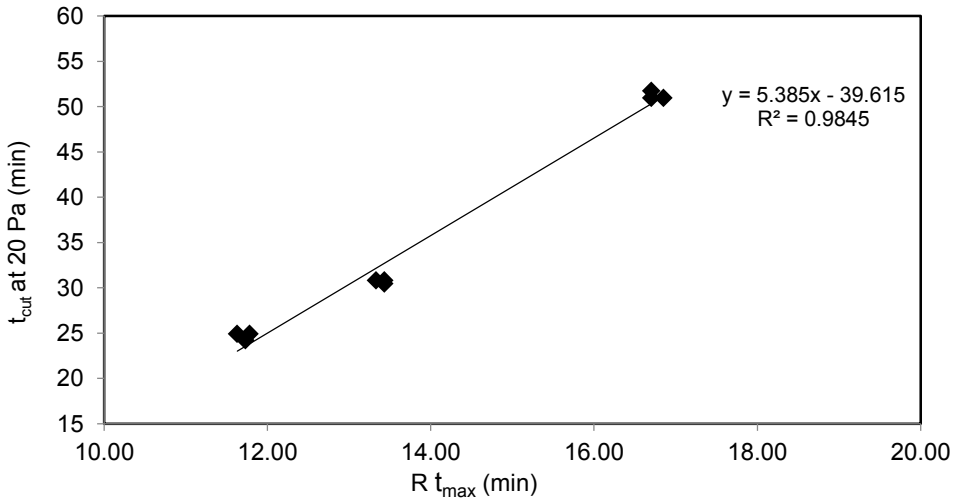

Figure 2. Linear correlation between the optical predictor t_{max} and cheese making indices $t_{G'20}$

Gelation occurs by formation of polymers of casein micelle due to cross-linking which can be monitored by NIR spectroscopy. These results confirm that gel strength and cutting time can be predicted from the light backscatter profile and milk coagulation can be monitored using NIR spectroscopy.

Conclusion

NIR light backscatter technology has the potential to determine the gel strength and predict the cutting time of enzyme induced milk coagulation. NIR sensor can be effectively used for real-time estimation of curd firmness which will facilitate in automation of cheese plants. Effect of different processing parameters on rennet induced milk coagulation can be successfully investigated by NIR spectroscopy.

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THE POTENTIAL OF UV-VIS SPECTROSCOPY AND CHEMOMETRICS FOR ADULTERANT DETECTION IN VODKA

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Abstract

Vodka is produced from ethyl alcohol sourced from an agricultural origin that has been produced *via* fermentation. The potential of UV-Vis spectroscopy and chemometrics for adulterant detection in vodka was considered. A range of potential adulterants were investigated including methanol, ethanol and water. A multivariate calibration model was developed for adulteration detection using PCA. Vodka samples were successfully categorised as both authentic or adulterated when UV-vis spectroscopy and chemometrics. This model has the potential to be useful for government agencies, beverage companies or other stakeholders to further enhance their control measures currently used by production industries.

Introduction

Vodka is a clear spirit which despite multiple distillation and filtration processes, the ethanol content will contain other trace elements such as methanol, esters, aldehydes and acetic acid. Regarding this fact, it is necessary to monitor the composition and verify the authenticity of the vodka being produced. There are many brands of vodka that are internationally recognised products with high quality and unique flavours. Unfortunately due to this success many of these spirits are subject to imitations and counterfeit. Common adulterants used in Vodka include ethanol, methanol and water. More adulterated spirits are popping up in the market that attempt to capitalise the reputations of huge labels that have been built over years of hard work. These counterfeit products then compete with the authentic brands. By its criminal nature, it is difficult to quantify the scale of illicit and counterfeit spirits sold in the market today, it is estimated that up to 30% of the spirits sold on the market contribute to 30 % of the revenue generated ("Spirit Europe", 2017). This has a direct negative effect on government revenue, the consumers trust is clouded with doubt, brand reputation is destroyed and on a more serious note it poses a huge public health risk due to substances added are unfit for human consumption. During the production of vodka, methanol and ethanol exist in safe quantities. However, adulterated drinks often skip multiple quality control tests. Toxicological studies have reported numerous counterfeit vodka samples found unsafe levels of methanol and ethanol greatly exceeded recommended limits following multiple hospital admissions. Each vodka sample will have a unique spectral fingerprint which will allow for the detection of any adulterants. These adulterants can be identified using software modelling and chemometrics principal component analysis (PCA). The main advantage of this technology is a non-invasive, rapid and accurate method to generate a chemical fingerprint of the bottles contents (Ellis *et al*., 2017).

The objective of this study is to differentiate adulterated vodka samples using UV-Vis spectroscopy and chemometrics techniques.

Experimental

Apparatus

UV-Vis instrument at the UCD School of Biosystems and Food Engineering laboratory will be used to obtain the spectral data. The PCA calibration models for the quantitative determination will use the online Unscarmbler X software (v10.5, CAMO Software AS, Olso, Norway).

Samples and adulterants

This work involves three different types of vodka from different geographical origins (Texas USA, Poland and Ireland) and will be used as calibration sets to construct chemometrics models. Two experiments will be carried out in the laboratory. First, a serial dilution will assess the influence of adding water at different ratios to the pure vodka samples will be analysed. Second, different levels of common adulterant (ethanol) will be added to the original pure vodka samples to see if they can be detected and distinguished.

Predicted results and discussion

Preliminary analysis of the sample spectra

Following the procedure described above, **Fig 1** shows the UV-Vis spectra of each of the non-adulterated vodka samples, showing relevant spectral information in the region between 200-400 nm and was therefore chosen to build the chemometric models. Pure vodka sample analyse will be used to create a database consisting of a set of analytical signals as a function of time that characterises the digital fingerprint profile of each sample. This database will be used to elaborate chemometrics models applied on the identification of each adulterated vodka sample.

Expected results

Sufficiently accurate quantitative PLS calibration models have been researched for whiskey and wine. Authentication of vodka samples will be assessed to see if it can be as successful using UV-Vis and chemometrics.

In the present paper by (Pontes *et al*., 2006) the classification of distilled alcoholic beverages (whiskey, brandy, rum and vodka) and verification of adulterants using near infrared spectroscopy (NIR). The results from the former study were successful and UV-Vis spectroscopy method is expected to perform in a similar manner.

The expected results will be similar to those presented in the paper published in the National Centre for Biotechnology Information (NCBI) by (Martins *et al*., 2017) where adulterated whiskey brands were successfully identified by UV-Vis spectroscopy and multivariate data analysis.

Modern spectroscopy techniques have recently been used to identify the content of spirits on a molecular basis through the packaging without opening the bottles. This non-invasive technique is a huge step forward in the battle against counterfeit spirits (Nordon *et al*., 2005). This research aims to see how successful the chosen spectroscopy method is with the battle against adulterated vodka.

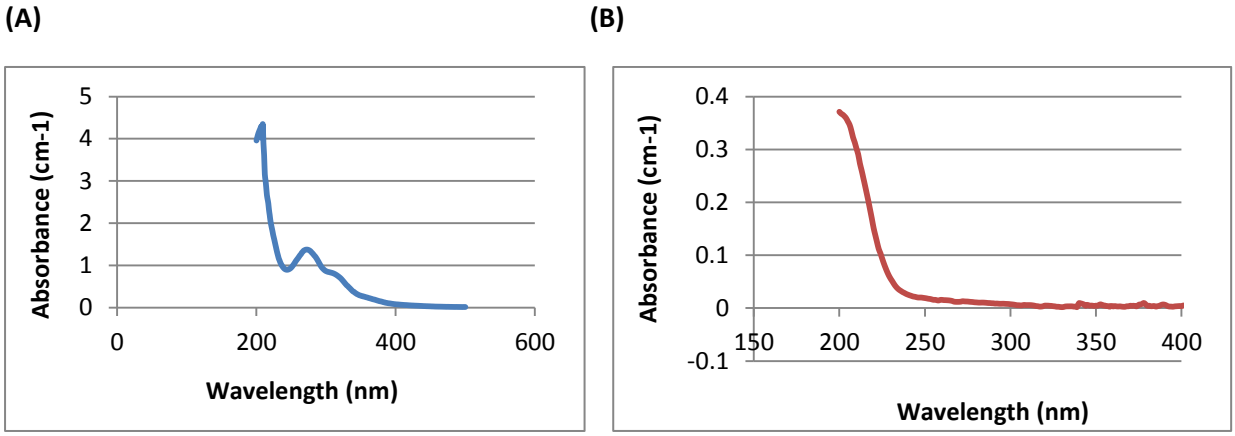

Figure 1. Typical UV-VIS spectrum of vodka (a) brand 1 (b) brand 2.

Conclusion

Sufficiently accurate quantitative calibration models for alcoholic additives could be detected using UV-Vis and chemometrics for whiskey, gin and rum. This paper hopes to verify UV-Vis spectroscopy to be a suitable method for the determination of authentication of vodka.

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REUSING LIGHT PLASTICS AS INSULATION FOR STORAGE BOXES

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Abstract

Marine litter is accumulating in oceans and adversely affecting the ecosystem and is also seeping into the food chain. The litter is composed largely of various types of plastic material. Hence, the possibility of using used light plastics as insulation for storage boxes is being tested. A minimally processed design approach has been adopted. The design assumes that the use case is during storage and transportation of quickly perishable foodstuffs namely fresh produce such as horticultural products and seafood. The most important part of this type of experimentation is the process of designing the insulation. Hence this paper will focus on the various designs used to create insulation out of light plastics with minimal processing. The design will be tested using an inferential statistical method called *t* test. It will be tested against various controls using a combination of parameters and environmental conditions to arrive at suitable inferences. The conclusions will be focused around the design of the insulation.

Introduction

Marine litter is said to be largely made up of plastics. The light plastics present in that would be the kind used in packaging of foods products. They are generally light in weight and have thickness in mm. The reason for the focus on light plastics is due to the increasing nature with which they have found their way into the oceans and the ease with which they might be ingested by aquatic animals and enter the food chain. As of March 2018, there are many reports of a massive marine litter dump found in the Pacific Ocean which is constantly increasing in size known as the Great Pacific Garbage Patch (Lebreton *et al., 2*018). Cleaning up procedures tend to be difficult since no particular country can be considered responsible due to its geographical location being in the middle of the ocean. Standard methods and resources to quantify the amount and its characterization are limited and require further development which increases the need for plastics to find other uses instead of being considered waste (Avio *et al.,* 2017). There are no set procedures to search for similar patches that might be currently growing which then raises the question of the various such marine litter sites that are yet unknown.

The process of reusing light plastics is a matter of bringing certain changes to the life cycle of these plastics. Where change exists, innovation follows. Innovation can be defined as the outcome of a process of value creation. It involves the process of changing the set of variables described in any system (Yezersky, 2007). In any innovation, the design is the most significant part of the process since the method of production will be based on this design. In order for the change and innovation to take place, the first step in the process is to design the new method or product that is being introduced. Since the steps following the design are completely based on whether the design is accurate, the process of design is the significant step for innovation. Among the various types of plastic that can be found in marine litter, light plastics can be used with minimal processing as compared to other materials such as plastic bottles which need certain amount of reshaping and moulding to be reused. Hence, it is worth taking a look at design ideas that can provide a process to reuse plastics that are being thrown away.

The objective of this study is to design insulation that can be used in a storage box from used light plastics with minimal processing involved.

Materials and Methods

Design of insulation

Light plastics will be collected in the form of food packaging from household sources for this experiment. A few different types of designs have been considered. Details such as the thickness and surface area of the insulation are calculated based on the current standard box sizes. The first design is to have many layers of the plastic pressed on top of each other till it reaches the required thickness. The second design involves introducing air packets into the layers of plastic. Certain designated points along the horizontal surface will be melted through to create air pockets between the layers present below. This will allow for control on the amount of air present in between the layers. The designs will be tested out against two cases having different controls.

According to Food Safety Authority of Ireland, transport and distribution of cold food should be done at temperatures of 5 °C and below. Refrigerated and non-refrigerated transport conditions will be mimicked using different temperature ranges. Hence, there are many different combination of parameters and environment in which the insulation will be tested.

Testing will be carried out as per a standard statistical *t* test. This test requires large amount of data for better accuracy. The data that will be collected is the temperature at every predetermined interval of time. The overall time period is considered based on the use case of the insulation which for fresh produce and will be 24 to 48 hours. This is a significant amount of time for fresh foodstuffs. It also allows enough time for the repetition of the procedure. The statistical analysis requires a large degree of freedom for higher accuracy. An independent t test will be conducted where the degree of freedom n will be $n < 25$. (Pandis, 2015a)

Statistical method of analysis

The method of analysis is an inferential statistical method called a *t* test. There are various types of *t* tests based on the analysis to be undertaken and the type chosen for this paper is the independent *t* test. This *t* test is conducted when comparing two independent groups by determining their means. The groups of data are assumed to be normally distributed. It considers the hypothesis that there is no statistically significant difference between the two sets of groups. The sample size considered is referred to as degrees of freedom. Each set of data boils down to a T value which is the difference in the data points of the group. From this, a P value is calculated which ranges from 0 to 1. A P value less than 0.05 represents that there is a significant difference between the groups and hence it rejects the null hypothesis. Hence in order for the test to prove the hypothesis true, the P value must be larger than 0.05. (Pandis 2015b)

The major parameters of the insulation in the design are the surface area covered by it and its thickness. Usually for insulations in buildings, various materials are layered together to form the insulation layer. It is done to provide better support to the layer and for other considerations in a building. For a storage box, the insulation needs to be able to provide protection from heat variations and it is considered to be working effectively by testing the quality of the food products kept inside. Hence, there will be two different controls in this experimentation process.

Case 1: The first control will assume the condition of no insulation. The *t* test will be conducted to check for a significant difference between the designed insulation and a situation of no insulation. The null hypothesis that there is no significant difference must be rejected in this case to show that the insulation is working effectively.

Case 2: The second control will a cool box that is used currently for the purpose of storage of food products. Here, the *t* test will be conducted will be between the designed insulation and a

current standard storage box to check for no significant difference. Hence, the null hypothesis that there is no significant difference between the two samples of data must be accepted.

Based on the results determined by the statistics, inferences can be made towards the design of the insulation. Since more than one design will be tested, a recommendation towards a better, more suitable design type can be made along with a comment on the environmental conditions.

Results and Discussion

The main results obtained will be the inferences derived from the statistical testing. These inferences will be decided based on the numerical end results of the various tests carried out. The T value and more importantly the P value will determine if there is no significant difference between the insulations being tested. Depending on the P value obtained, the null hypothesis will be accepted or rejected for each case. As this is a numerical statistical analysis, it is not a binary 1 or 0 solution. The amount of difference is also significant as it helps to decide the difference in the set of samples considered as well. The type of experimentation involves a large number of repetitions and hence the few changes that can be made as a result of the experimentation will be towards the design of the insulation rather than the design of the experimentation process.

The testing done here is using only light plastics whereas in general, other substances are also present in insulations that are used as support and fillers. Further studies can be recommended that involve these support materials such as cardboard, fibre glass and glass wool. It is also important to note that these results are true for a specific set of experimental conditions and can change subject to change in these parameters such as temperature difference, time period of consideration and materials present in the insulator.

Conclusions

The main conclusion will be towards whether this design of insulation suitable to provide effective insulation for a short period of time. If the conclusions are significantly positive, a new method of usage of light plastics can be planned using this design as a base. It could find application in storage and transportation of easily perishable food products and can help reduce the postharvest losses that occur during transportation and storage.

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INVESTIGATION OF THE EFFECT OF THAWING ON SALMON FILLETS USING TIME SERIES HYPERSPECTRAL IMAGING (TS-HSI)

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Abstract

As a rapid and non-destructive analysis technology, hyperspectral imaging (HSI) has been widely used in food industry. This study was carried out to investigate the effect of three different thawing methods (air thawing, microwave thawing, and freeze thawing) on salmon using a near infrared (900-1700 nm) time series hyperspectral imaging system (TS-HSI). Principal component analysis (PCA) was applied to explore the spectral change during the thawing process and partial least squares discriminant analysis (PLS-DA) was used to discriminate salmon fillets suffered from different thawing methods. This study confirmed the potential of TS-HSI for investigation of changing characteristics of salmon fillets over time sequences using different thawing approaches.

Introduction

Salmon is regarded as a kind of healthy fish, which is rich in protein, omega-3 fatty acids, vitamin, and cholesterol (a range of 23-214 mg/100 g). Unsaturated fatty acids can effectively reduce blood fat and blood cholesterol and prevent cardiovascular diseases. Astaxanthin is a kind of superior antioxidants, which can effectively remove oxygen free radicals and enhance cell regeneration. Omega-3 fatty acids are indispensable substances in the brain, retina, and nervous system, which have the effect of enhancing brain function, preventing Alzheimer's disease, and preventing vision loss (Isaksson *et al*., 1995).

Frozen storage is currently one of the most respected methods of food preservation, which can ensure the food's flavour and nutritional value to the greatest extent (Delgado and Sun, 2001). The quality changes of salmon in the process of freezing and thawing are mainly reflected in three aspects: quality characteristics, physical changes, and chemical changes. During thawing process, the ice crystals in the product melt into water, and the part that cannot be absorbed flows out of the tissue called juice loss. The reason for this is the mechanical damage to the muscle tissue structure by the formation and growth of ice crystals during the freezing process. Meanwhile, weight loss occurs during the freezing process, because the ice crystal state is sublimated from the surface of the frozen product (Alizadeh *et al*., 2007). Different thawing methods have different effects on salmon.

Hyperspectral imaging is a rapid, accurate, and non-destructive technique applied in the quantitative determination of food, which can provide two-dimension spatial and one-dimension spectral information of the object by integrating imaging and spectroscopy techniques (Gowen *et al*., 2007). For a hyperspectral image, each pixel corresponds to a spectrum to provide both external quality features and internal structural features.

Principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) were used in this study. **The objective of this study was to investigate and distinguish the effect of three different thawing methods on salmon fillets using near infrared (900-1700 nm) time series hyperspectral imaging technology.**

Materials and Methods

Salmon sample preparation

Salmon fillets originated from a farm in Ireland were labelled and then frozen stored at laboratories of Food Refrigeration and Computerized Food Technology (FRCFT), University College Dublin (UCD), Ireland. Each salmon fillet was divided to about 200 grams in different sizes and no any two fillets were cut from the same fish.

RGB image acquisition

Computer vision means using cameras and computers instead of the human eyes to identify, track and measure the machine vision. An RGB image of each sample is acquired using computer vision before each scanning, which consists of a high-pixel camera and a computer installed RemoteCapture DC software.

Hyperspectral image acquisition and calibration

The hyperspectral imaging system used in this study consists mainly of an illumination unit (two 500 W halogen lamps), a spectrograph with the wavelength range of 900-1700 nm with a spectral resolution of 3.34 nm (record 256 bands for each spectrum), a C-Mount CCD camera, translation stage, and a computer installed hyperspectral image acquisition software (Spectra SENS). This system was turned on and allowed to stabilize for around 30 min before scanning. After removing noisy wavelengths and selecting regions of interests (ROIs), the hyperspectral image of each sample is ready for follow-up processing using MATLAB.

Multivariate exploration

Data acquired by the hyperspectral imaging system is a hyperspectral cube or a "hypercube". Each hypercube usually comprises of thousands of spectral signature distributed over the measured area, which requires multivariate exploration to obtain the required information. In this study, PCA is used to summarise and explore the useful information contained in a hypercube, which produces principal components (PCs) that retain as much of the original variable information (for example variance) as possible and are not related to each other. PLS-DA is a linear parametric classification chemometric technique based on the partial least square (PLS) algorithm, and it is used to classify different thawing methods in this study.

Weight loss measurement

Weight loss of individual salmon fillet during thawing process was measured using a mass balance and presented as a percentage of weight loss compared to the initial weight of the frozen sample.

$$\mathrm{WL}(\%) = \frac{\mathrm{W}_{\mathrm{initial}} - W_i}{\mathrm{W}_{\mathrm{initial}}} * 100\%$$

where *i* represents time interval during thawing. It should be noted that the total thawing time is different for different thawing methods, *ie.*, 30 min for air thawing, 1 min for microwave thawing, and 60 min for freeze thawing.

Results and Discussion

Spectral feature analysis

Figure 1 shows the mean spectra of three different thawing methods at different intervals. The difference of reflectance values is related to the effect of different thawing methods and the change

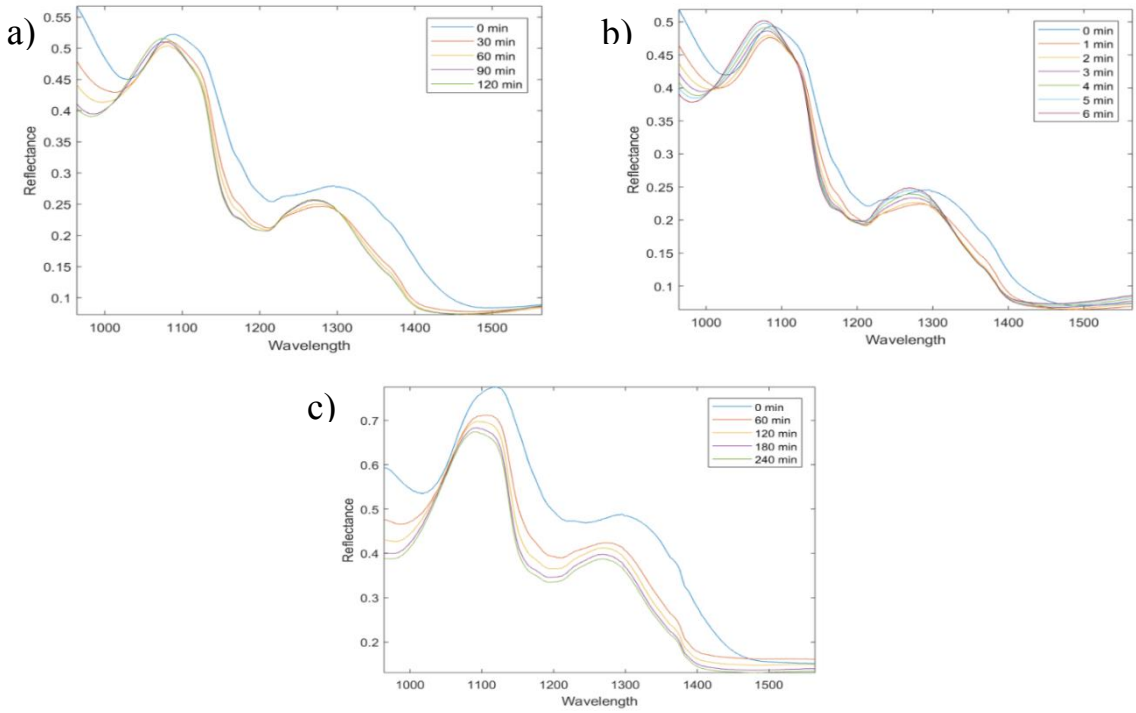

Figure 1. Mean spectra of salmon fillets by three thawing methods: a)air thawing, b)microwave thawing, c) freeze thawing.

characteristics during the thawing process. The near-infrared spectrum is an important and useful analysis method to analyse and distinguish different substances. Each trough corresponds to the absorption intensity of different substances. Intensive absorption peaks at around 970 nm (O–H stretching second overtones) and 1400 nm (O–H stretching first overtones) were related to the absorption of water content. While the absorption peak at about 1200 nm (C-H stretching the second overtone) was attributed to the fat content of salmon fillet (Xu *et al*., 2016).

Weight loss analysis

The weight loss result of each thawing method is shown in Table 1. The microwave thawing method has the largest weight loss when completely thawed, which is one kind of rapid thawing method allowed a large number of ice crystals to melt at the same time and no time to transfer, resulting in a lot of juice loss. Future studies are needed to determine whether weight loss can be used as a basis for distinguishing between three different thawing methods.

Table 1. Weight loss of three thawing methods

Air thawing		**Microwave thawing**		**Freeze thawing**	
Time	**WL**	**Time**	**WL**	**Time**	**WL**
0min	0.000%	0min	0.000%	0min	0.000%
30min	0.160%	1min	0.147%	60min	0.052%
60min	0.426%	2min	0.393%	120min	0.676%
90min	0.905%	3min	0.933%	180min	1.145%
120min	1.438%	4min	1.473%	240min	1.717%
		5min	1.866%		
		6min	2.259%		

multivariate exploration by PCA and PLS-DA (Expected)

Concatenated PCA of each sample during microwave thawing is carried out and the results are shown in Figure 2. Each PC image was rescaled and weighted according to its corresponding eigenvalues. Figure 2 visualizes the major changes in the thawing process. Regions of salmon, ice and fat are clearly discernable in the combined PC source images at each time point. The PC1 score images changing possible because the crystallization melts from the centre of the sample during microwave thawing. The PC loading reveals major variations around 1350 nm, which corresponds to water in salmon.

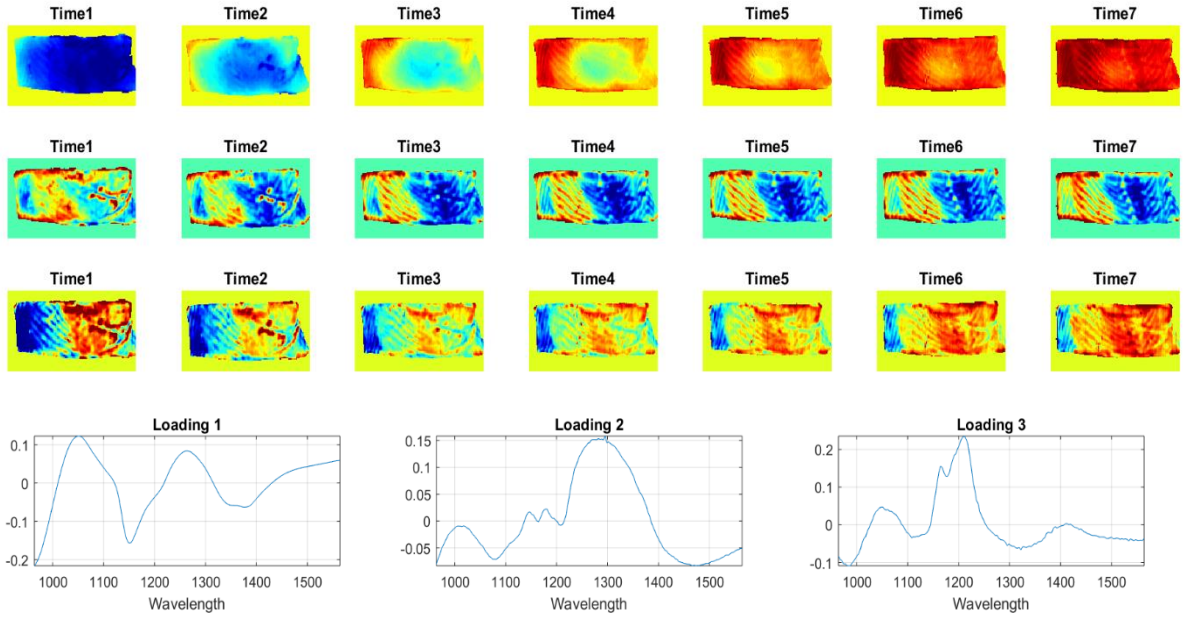

Figure 2. PCA results of microwave thawing method using MATLAB

Conclusions

This work suggested the potential and possibility of TS-HSI as a rapid and non-invasive technique for detecting the change during thawing process and distinguishing three different thawing methods.

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OBJECT RECOGNITION FOR WASTED FOOD
A BRIEF REVIEW

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Abstract

Object recognition technology has been increasingly used in all aspects of our lives work and security. Therefore, object recognition has important research significance, and the obtained research results have very broad application prospects. In recognizing food in dishes, Feature-based object recognizers generally work by pre-capturing a number of fixed views of the object to be recognized, extracting features from these views, and then in the recognition process, matching these features to the scene and enforcing geometric constraints. Generally speaking, food waste is happening during any stage of the food supply chain. This study demonstrates the potential of using imaging processing technology to decease the food waste in consumer stage by analyzing individual food intake and eating habits.

Introduction

Despite the changes in posture, illumination, and occlusion, the ability of humans to identify thousands of object categories in cluttered scenes is one of the most surprising capabilities of visual perception, which is still unmatched by computer vision algorithms.(Oliva et al.2007) The initial state of the computer can only identify the basic information on the pixel point. This is the same as the biological vision. The reason that the organism can distinguish the object is because the biological neural system processes the original image. The computer image recognition is also a process of logically classifying the original optical information.

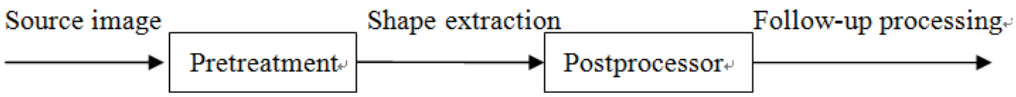
Object recognition is used in many different applications and algorithms. The common process for most schemes is that, given some knowledge about the appearance of certain objects, to examine one or more images to assess which objects are present and where they exist. However, each application has specific requirements and restrictions. This fact has led to a rich variety of algorithms (Treiber *et al*., 2010).

Normally, when a person finishes eating, it is difficult for us to use our eyes to measure how much food we have left. And the amount of wasted foods can be used in many places. So we can use an object recognition program to estimate how much food each person has left, then to estimate the average food intake in different groups in terms of age, gender and region. At the same time, these data can be used in recommending restaurant supply proper amounts of food which can reduce food waste in general.

The objective of this study is to identify how much food is wasted by one meal through object recognition and provide an assumption to use this technology to decease the food waste.

Materials and methods

Shape extraction
The process of extracting shape:



Pretreatment: Grayscale Transformation
In processing, the gray level occupied by the original image data is changed while it will not change the mutual spatial relationship between image pixels.

Shape segmentation: Edge Detection
Because the differential operator has the effect of highlighting the change of gray scale, the differential operation of the image, the gray level at the edge of the image changes greatly, so the differential calculation value is higher at this point, and these differential values can be used as the edge intensity of the corresponding point. Edge points are extracted by threshold discrimination. For example, if the differential value is greater than the threshold, it is an edge point.

Shape feature extraction
Through the pre-processing of the image, we obtained the shape of the target. In order to further analyze and identify the target, the correct conclusion must be obtained by quantitatively and qualitatively analyzing the shape of the target. These conclusions are based on the shape of the target. In order to identify a target, we must describe the shape of the target, that is, extract some features of the shape to represent the target. Stylianou and Farin (2003) provide a method called crest lines to automatically extract shape features that they will use in a later work to construct a feature based object comparison.

3D object recognition
One common problem with image-based recognition is to detect the 2D shape of the object in the image, i.e. to find the relevant image area. Recent methods for detecting objects in an image typically involve scanning the entire image at different scales to obtain an object-specific image pattern, and then using a classifier to determine if the area is relevant. The latest developments show the use of support vector machines (SVMs) to accomplish this task. A key element is the extraction of image features, i.e. part of the image, such as corners, edges, and other points of interest. This is usually done using a correlation-based approach using templates or edge-based methods that use image gradients (Solem et al. 2015)

Image J
Image J is a public domain, Java-based image processing program developed at the National Institutes of Health. Image J uses an open architecture design that provides extensibility through Java plugins and recordable macros. (Girish et al. 2004) Image J can display, edit, analyze, process, save, and print 8-bit, 16-bit, and 32-bit images. It supports TIFF, PNG, GIF, JPEG, BMP, DICOM, FITS and many other formats. Image J supports image stacking, which is a multi-threaded stacking of multiple images in a single window and parallel processing. As long as memory is allowed, Image J can open any number of images for processing. In addition to basic image manipulations such as scaling, rotation, warping, and smoothing, Image J can also perform image area and pixel statistics, spacing, angle calculations, create histograms and profiles, and perform Fourier transforms.

Sharpen in Image J
The arithmetic in this part is increasing contrast and accentuating detail in the image or selection, but may also accentuating noise. This filter uses the following weighting factors to replace each pixel with a weighted average of the 3 × 3 neighborhood:

$$\begin{matrix} -1 & -1 & -1 \\ -1 & 12 & -1 \\ -1 & -1 & -1 \end{matrix}$$

Find edges in Image J
The arithmetic in this part is using a Sobel edge detector to highlight sharp changes in intensity in the active image or selection. Two 3 × 3 convolution kernels (shown below) are

used to generate vertical and horizontal derivatives. The final image is produced by combining the two derivatives using the square root of the sum of the squares.

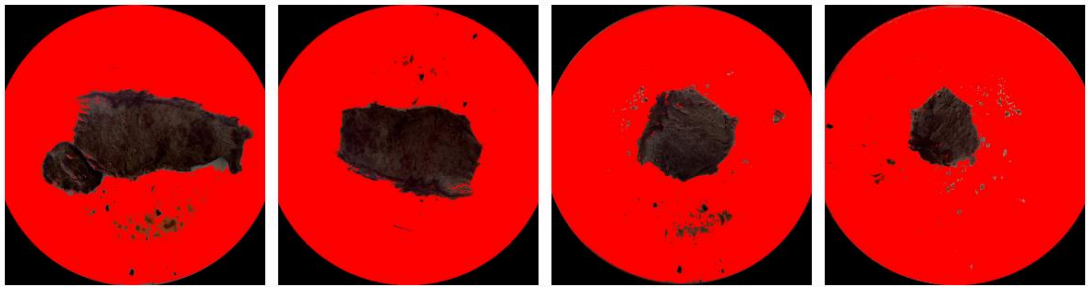
$$\begin{matrix} 1 & 2 & 1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{matrix} \qquad \begin{matrix} 1 \\ 2 \\ 1 \end{matrix} \qquad \begin{matrix} 0 & -1 \\ 0 & -2 \\ 0 & -1 \end{matrix}$$

Results and Discussion

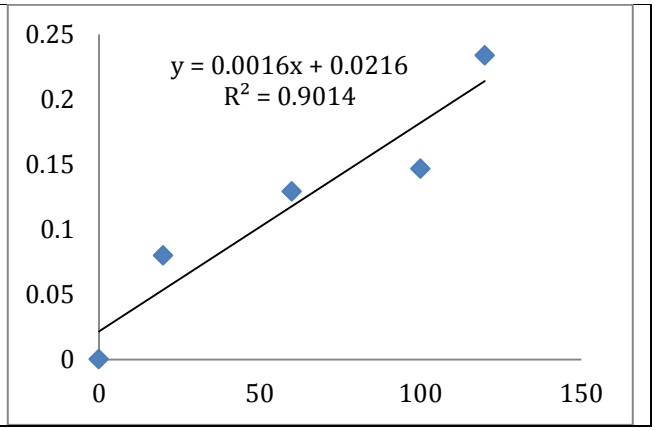
The first step

The proportion of wasted food was estimated by identifying the object of a single food with regular shape and then analyzing the area of the food before eating and the left food after eating through analyzing the ratio of the area of the food and plate. However, the food with regular shape and uniform density is supposed to have a good correlation in area and weight. Generally speaking, one meal usually has mixed foods and complicated density distribution, so it will be difficult to measure how much food is wasted by vertical pictures.

Data analysis



Area (ratio)	Food(g)
0.2336	120
0.1464	100
0.1289	60
0.0799	20
0	0



As we can see from the pictures and charts, the area of steak and the weight of food have a relative high standard deviation. Thus, this model can be used to predict the quality of steaks and similar foods through single pictures. As a result, it is possible to analyze one or two foods with uniform density and regular shape by using the volume and color in the same time. If the restaurant has this technology to record the food intake of different customers, the restaurant can provide foods corresponding to the customer's food intake when the same customer has the same food next meals. I will decrease the food waste by one customer with one meal.

However, one meal always contains more than two ingredients and other unstable factors like sauces. Therefore, this model needs additional parameters to correct. In this respect, a 3D model of the food being tested is built from different views, and the software algorithm is optimized so that the amount of wasted food can be estimated through pictures.

Second step

If the customer can take photos of the food in different views before and after eating meals, this model can analyze the customer's food intake, and record dietary preferences. Then, collecting data based on each person's food intake and eating habits and sharing this data with each restaurant. When a restaurant provides foods that meets the customer's food intake, thereby avoiding waste. This method can also be applied to every family to avoid wasting food by cooking too much food.

If everyone uses this model to record the food they eat every day, and analyzes each person's diet and nutritional balance through an object recognition program, and proposes a nutritional diet plan, it will not only help reduce food waste, but also plays a supporting role to a healthy life.

Conclusion

This study provides good models to analyze the percentage of wasted food through pictures. With deeply researching this study, it can theoretically solve part of the problem of food waste, and it has a very meaningful prospect for national healthy diet.

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MONITORING OF ACID INDUCED MILK COAGULATION KINETICS USING NIR SPECTROSCOPY

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Abstract

This study investigated near-infrared (NIR) spectroscopy as a process analytical technology (PAT) to monitor acid induced coagulation kinetics of skim milk under different concentrations of glucono-δ-lactone (GDL). Rheometry was used as a reference method for milk gel strength and firmness measurements. Durations required for storage modulus (G'), a unit for milk gel strength and firmness, reaching 2 Pa were recorded during the coagulation experiments. By comparing two sets of data gained from two methods, the results demonstrated that there was a 97% correlation between the NIR spectral parameter and time required for milk gel to reach target storage modulus. Finally, the conclusion gives a brief summary that NIR spectroscopy has a potential in real-time monitoring for kinetics of acid induced milk coagulation process. Thus, the effectiveness of evaluation for dairy manufacturing process could be improved in the future (Panikuttira *et al.*, 2017).

Abbreviation key: NIR = near-infrared, **GDL** = Glucono-δ-lactone, **G′** = storage modulus.

Introduction

As a non-destructive inspection method, NIR spectra shows sample results based on their physical properties. The sample could be measured within a short period in seconds by either reflectance or transmittance, and data gained from the measurement could be processed with mathematical modelling. In this way, some contents or quality attributes in food products can be determined. (Osborne, Fearn and Hindle, 1993)

Milk coagulation is the primary step in the production of many dairy products, such as cheese and yoghurt. This process can be induced by acid or rennet. In acid induced milk coagulation procedure, based on the reduction of pH in milk, colloidal calcium phosphate (CCP) can be solubilized from casein micelles (Herberg *et al.,* 1999). Afterwards, casein association lead to gel formation (Herberg *et al.,* 1999). During the acid coagulation of casein micelles, hydrophobic effects are the major driving force of protein-protein interactions (Herberg *et al.*, 1999). The rheological properties of milk gel could be determined by the kinetics.

In this study, a combined NIR-fluorescence was applied to evaluate the milk coagulation processes, as the reflectance data could be used for monitoring milk gel particle size distribution and modification (Panikuttira *et al.,* 2017). Due to the larger particles formed caused by casein micelles aggregation, there is a modification in particle size distribution which could enhance the NIR reflectance in milk coagulation process (Panikuttira *et al.*, 2017). Thereby, NIR reflectance data were recorded during the milk coagulation processes at different levels of GDL and compared to the rheological parameter (G') for the result analysis.

The objective of this study was to investigate the use of NIR spectroscopy to monitor acid induced milk coagulation kinetics

Materials and Methods

A 12 L laboratory jacketed vat with a combined NIR-fluorescence sensor mounted on the side wall was applied for milk coagulation experiments, and skim milk with 3.5% (w/v) protein and 0.3% (w/v) fat bought from the local supermarket was used. For acid coagulation process, different concentrations of GDL were applied.

Real-time NIR reflectance data of coagulation process was obtained from the combined NIR-fluorescence sensor on line. In contrast, a rheometer was chosen as a reference approach for measurement of acid coagulation kinetics, which could obtain milk gel strength and firmness.

Reflectance data collected by the combined NIR-fluorescence sensor was derived. The time matches the maximum value of the first derivative curve for each experiment was marked as Rtmax. The time required for milk gels to attain storage modulus of 2 Pa was recorded according to the monitor by rheometer as well. By comparing Rtmax with the time needed for milk gel to obtain a 2 Pa storage modulus, a correlation could be found.

Results

The concentration of GDL had direct effects on reduction of pH in milk and the rate of coagulation. Measurement results from NIR spectroscopy were notably different based on varies levels of concentration of GDL added.

For each experiment based on different GDL level respectively, the optional response ratio at 880 nm obtained from NIR - fluorescence sensor against time variation could be plotted as an example shown in **Figure 1**, and the first derivate and second derivative of the optical response ratio were plotted as well. Time matches the maximum value of first derivative curve for the experiments were defined as Rtmax.

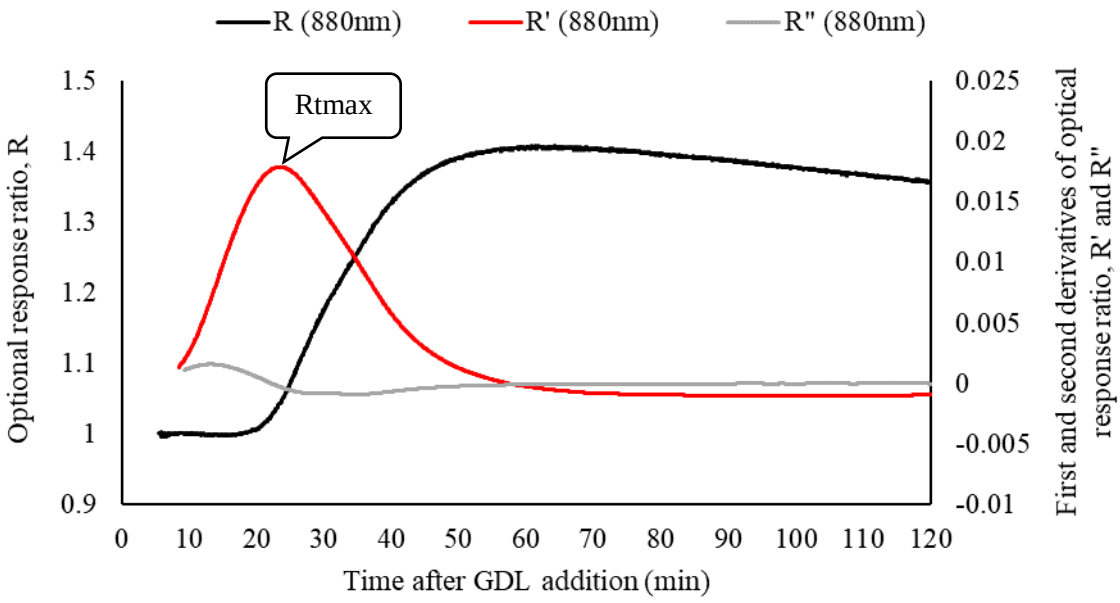

Figure 1. Optional response ratio R, and its first and second derivatives (R' and R") with time.

Times required for milk gel to reach 2 Pa of storage modulus were gained from controlled experiments, which were data detected by the rheometer. Results gained from those two approaches were correlated with time as shown in **Figure 2.** It was demonstrably that there

was a 97% correlation between Rtmax gained from combined NIR – fluorescence sensor and time corresponding to the storage modulus of 2 Pa obtained by the rheometer.

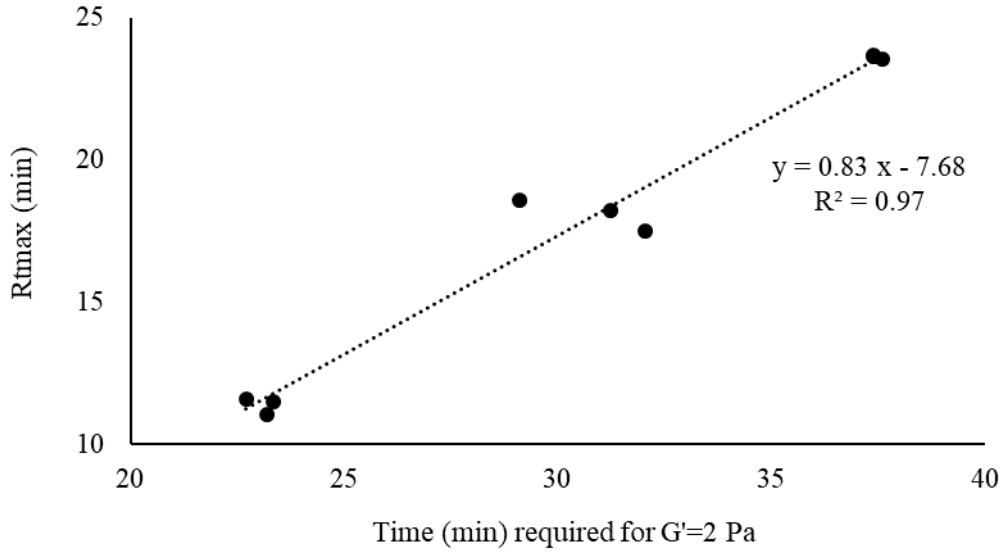

Figure 2. Comparison of prediction with the actual time corresponding.

Conclusions

According to the results, there was a 97% correlation between Rtmax gained from combined NIR – fluorescence sensor and time corresponding to the storage modulus of 2 Pa.

Further studies on varies predictions models in processing reflectance data obtained from NIR spectroscopy as a process analytical technology (PAT) tool in the dairy industry could be carried on. Thus, monitoring of coagulation process by detecting milk coagulation kinetics can be more accurate and real-time controlled in the future.

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ASSESSMENT OF INFANT FORMULA QUALITY AND COMPOSITION USING VIS-NIR AND CHEMOMETRICS

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Abstract

In this study, the visible and near-infrared (Vis-NIR) analysis techniques combined with chemometrics tools were used to predict infant formula quality and composition parameters. This included preheat temperature, storage temperature, storage time, and advanced fluorescence Maillard Product and soluble tryptophan (FAST) index, soluble protein, fat and surface free fat (SFF) content. A preheating temperature prediction model for infant formula was established using Partial Least Squares Regression (PLS) and Principal Component Regression (PCR).

Introduction

Infant formula contains the corresponding nutrients and bioactive ingredients that babies need in the process of growth. It aims to meet the nutritional and health needs of infants and to be a suitable substitute for mother's breast milk (Desic *et al*., 2011; O'Callaghan *et al*., 2011) The manufacture of infant formula involves multiple processing steps, including the use of water mixed ingredients to obtain a homogeneous solution, and then fully heat treatment or dehydration to provide bacteriological safety (O'Callaghan *et al*., 2011). The heat treatment usually used in the production of infant formula includes pasteurization (72 °C), high temperature short time (HTST) heating, ultra high temperature (UHT) treatment (135-150 °C) and container sterilizing (115-120 °C) (Desic *et al*., 2011; O'Callaghan *et al*., 2011; Crowley *et al*., 2016). However, heat treatment may lead to the major physical and chemical changes in the infant formula, including protein denaturation and aggregation, lipoprotein and protein interaction, sugar isomerization and Maillard reaction (Desic *et al*., 2011; Crowley *et al*., 2016). Infant formula is usually packaged, transported, stored and distributed in cans. Although milk powder usually has a longer shelf life at ambient temperature (12-24 months), the infant formula powder made with vegetable oil or rich polyunsaturated long chain fatty acids has a lower storage stability (Tham *el al*., 2017; Cheng *el al*., 2017). It has been shown that higher storage temperatures can accelerate the deterioration of infant formula quality because in most cases physical and chemical reactions increase at higher storage temperatures (Cheng *et al*., 2017).

The preheating process could lead to the degeneration and aggregation of milk protein, and the changes in carbohydrates, including the isomerization of lactose, degradation and Maillard browning reaction (Patel *et al*., 2007; Ayala *et al*., 2016). Visible near infrared spectroscopy (Vis-NIR) is a mature, fast and nondestructive vibrational spectroscopy technology. It has become one of the most popular analysis methods in the food industry. In recent years, NIR has been widely used for the analysis of dairy products (Aernouts *et al*., 2011, Inácio *et al*., 2011). **The objective of this project was to study the combination of Vis-NIR spectroscopy and stoichiometry to establish a rapid and non-destructive method for quality and compositional testing of infant formula milk powder samples**.

Materials and Methods

Materials
The skim milk powder (SMP) was prepared by fresh raw milk obtained from the dairy farm of Teagasc (Moorepark, Cork, Ireland). It was skimmed at 50 °C, evaporated to 30% total

solid (TS) at 60 °C, and at the inlet and outlet temperatures of 180 °C and 95°C at the single stage spray dryer. Whey protein concentrate (WPC 35%w / W protein) was obtained from Arrabawn Co-op Society Ltd. (Nenagh, Co. Tipperary, Ireland). Vitamin and lactose are provided by Glanbia (Kilkenny, Ireland). Sunflower seed oil is purchased from a local supermarket (Supervalu, Fermoy, Ireland).

Use 4.1 kg SMP, 5.5 kg WPC, 13.8 kg lactose, 5.9 kg sunflower oil, 0.301 g vitamin A, 0.670 g vitamin B and 60.7 kg water to make model liquid infant formula mixture. Using MicroThermics Lab heat exchanger (MicroThermics, North Carolina, USA) at a flow rate of 2 L min−1 with a holding time of 15 s to preheat the mixture of the Model liquid infant formula mixes at three different temperatures (72, 95 and 115 °C). An in-line two stage valve-type homogeniser (150/50 PSI) (Model NS2006H, Niro Soavi, Parma, Italy) was used to homogenate the preheated samples at 65 °C.

Following overnight storage at 4 °C with gentle agitation, using a single-effect falling film evaporator to evaporate the samples were in recirculation mode at 65 °C to 50% TS (Anhydro F1 Lab; Copenhagen, Denmark), then using an Anhydro 3-stage drier with fines return to the top of the drier (SPX Flow Technology, Soeborg, Denmark) start spray drying. Inlet/outlet temperatures of the spray dryer were set at 175/ 90 °C respectively.

Infant formula samples were initially manufactured at room temperature (~20 °C) (0 months storage) and then analysed at two different temperatures, namely 15 ± 2°C and 37 ± 2°C, for up to one year. Aliquots of samples from each storage regime were analyzed at 3, 6 and 12 months after production. Two experimental designs were repeated for 4 repetitions × 3 preheating temperatures × (0 months storage + (2 storage temperatures × 3 storage times)) (n = 84).

Vis-NIR spectroscopy
The Vis-NIR spectra were collected on the NIRSystems Inc. (Maryland, USA) NIRSystems 6500. The infant formula was filled into the ring glass with diameter of 5.5 cm (7.5 cm diameter and 1.5 cm depth) and sealed with a screw cap. The reflectance spectrum (log (1 / R)) of logarithmic transformation is obtained and recorded in the spectral range of 400-2498 nm based at 2 nm steps. Two sub samples were scanned for each sample. All samples were scanned in random order at room temperature (~ 20 C). We use WINISI software (version 1.04, Infrasoft International, Port Matilda, USA) to do spectrum acquisition and file conversion. The Spectra is exported from WINSI software as a JDX file. In the subsequent stoichiometric analysis, the average value of 2 repeated scans per sample was used.

Chemometric analysis
The obtained NIR spectra were introduced into The Unscrambler software (v9.7; Camo, Trondheim, Norway) and the selected spectral range, i.e. 400-2500 nm (1050 wavelengths) were analyzed. Principal component analysis (PCA) was performed as an exploratory chemometric analysis using a spectral range. Partial Least Squares Regression (PLS) was used to predict the quality and composition of infant formula.

Expected results and discussions

Vis-NIR spectra
The spectrum of all infant formula samples is shown in Figure 1. It can be observed that the baseline variability of samples increased within the spectral range of 1100-2498 nm, and the spectra of 3 different preheating temperatures overlapped. There are a few sets of data at 1440-1944 nm. After consulting the relevant information, it is found that the storage conditions of the products affect the water content of the product during the experiment, and the water content of the product is higher than that of the other samples.

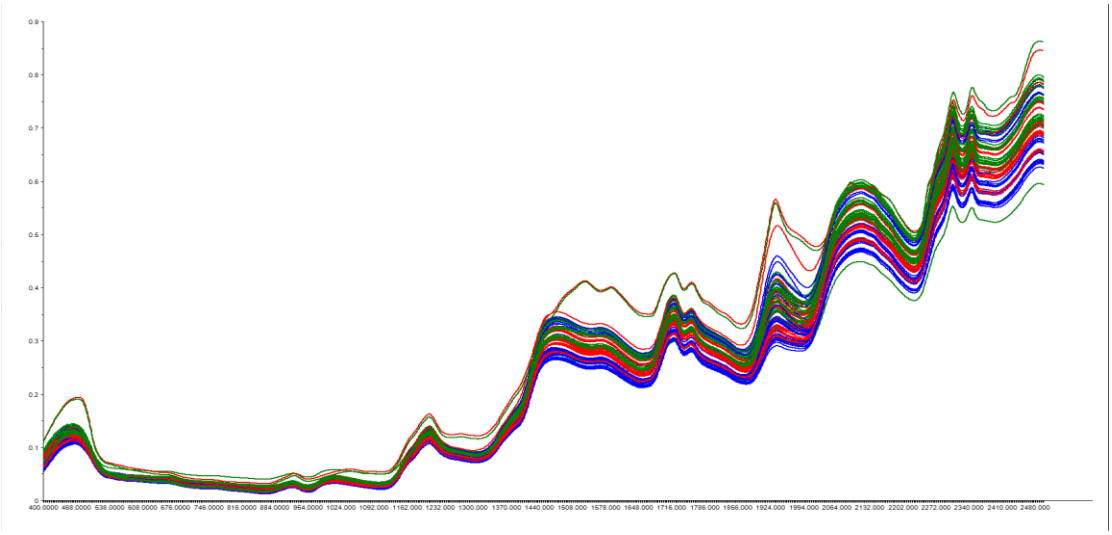

Figure 1: Log(1/R) Vis-NIR spectra of infant formula

Figure 2 shows PCA score plots of preheated samples based on the full spectral range. It can be seen that four sets of data are outside the standard circle. They are caused by excessive water content resulting in the deviation of its spectral data. In order to reduce the deviation of the final results, these data will be eliminated in the original spectral data before further using the PLS modeling for chemometrics analysis.

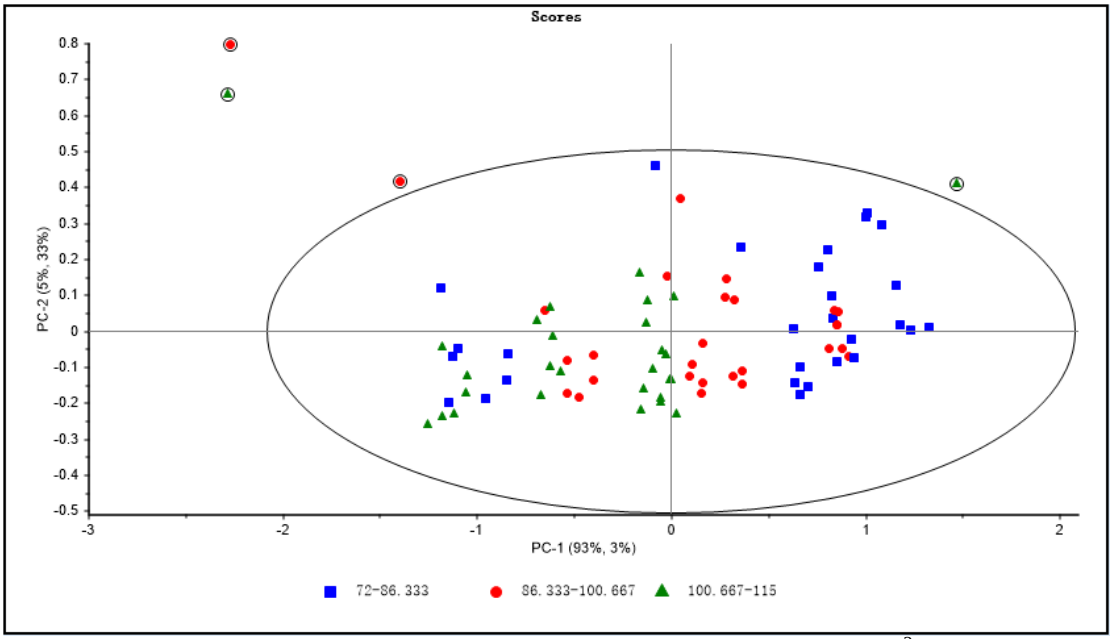

Figure 2: Scores plots of infant formula by using the Hotelling's T^2 ellipse

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Saif Shaikh, Ming Zhao

Project Title: Development of pat tools for the quantitative analysis of minerals in infant formulas

Project Leader: Professor Colm O'Donnell

Abstract

Commercially produced infant formulas are enriched with minerals and other nutrients that provide adequate nourishment among infants and toddlers (Soyeurt *et al.,* 2009). Therefore, quantification of mineral content in the infant formula during manufacturing process becomes a critical quality control attribute. This study investigated the potential of Process Analytical Technology (PAT) tools for the quantification of eight major elements i.e. Cu, Fe, Mn, Zn, Mg, Ca, K, and, Na in aqueous infant formula samples (n = 83). Inductively coupled plasma-atomic emission spectrometry (ICP-AES) and Fourier transform midinfrared (FTIR) techniques combined with chemometric approaches i.e. principal component analysis (PCA), partial least squares regression (PLS-R) and data fusion were used to build prediction models.

Step 1
The process of selection of reference methods for element analysis in aqueous infant formulas:

Selection of infant formula samples with different compositions ⇨ Selection of ICP-AES sample preparation method ⇨ ICP-AES analysis of the samples

Step 2
Evaluation of PAT tool for mineral element analysis in aqueous infant formulas

Analysis of samples using FTIR spectroscopy ⇨ Chemometric approaches for analysis for results ⇨ Develop PAT tools for quantitative mineral analysis of aqueous infant formulas

Preliminary PLSR analysis produced positive results. Coefficients of determination of cross-validation between the FTIR predicted and the measured values were 0.87, 0.84, and, 0.75 for Ca, Mg, and, K respectively.

This study proved the potential of the FTIR spectroscopy and chemometric tools to predict mineral contents. Further study will be conducted to build robust calibration models to predict other minerals in the aqueous infant formula.

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Soyeurt, H., Bruwier, D., Romnee, J.-M., Gengler, N., Bertozzi, C., Veselko, D., Dardenne, P. (2009) 'Potential estimation of major mineral contents in cow milk using mid-infrared spectrometry', *Journal of Dairy Science*, 92(6), 2444–2454, available: http://www.sciencedirect.com/science/article/pii/S0022030209705594.

Renxi Kang, BE, M.EngSc.

Project Title: Exploration of guided microwave spectroscopy (GMS) as a process analytical tool for mineral content determination in aqueous infant milk formula (INF) samples

Project Leader: Prof. Colm O' Donnell, Dr. Ming Zhao

Abstract

Guided microwave spectroscopy is a rotational spectroscopic technique, which is based on the determination of complex permittivity (ε) of a sample by creating a guided electromagnetic field in a frequency range of 0.25-3.2 GHz (Wellock and Walmsley, 2004). During the electromagnetic irradiation, polarization and depolarization of ions and molecule gives rise to their dielectric properties, which are dependent on the frequency range of electromagnetic field, the measurement temperature setting and the characteristics of samples(Zhang et al., 2014, Wellock and Walmsley, 2004). The current study explored the GMS system in combination with chemometric analysis as a process analytical tool for mineral determination in aqueous INF samples. Aqueous samples (n=83) were prepared in five concentrations (i.e. 3%, 5%, 8%, 10% and 13% w/w) using INF powder samples dissolved in deionized water. Samples were measured in 0-1200 MHz with 4 MHz increments at both 22 ºC, 50 ºC using the ε-scan in-line GMS analyzer (Thermo Fisher Scientific inc., Takkebijsters Breda, The Netherlands) at a static condition. The determination of minerals (i.e. Ca, Mg, Zn) in aqueous INF samples was carried out using the Inductively coupled plasma-atomic emission spectrometer (ICP-AES) (Vista Pro RL, CCD simultaneous ICP-AES, Varian, Victoria, Australia). The chemometric analysis were carried out using R (x64 3.3.2) studio with "pls" and "plsVarSel" packages. In this study, the PLSR models were developed to predict Ca (2.756-25.295 ppm), Mg (0.281-2.537 ppm), and Zn (0.085-2.575 ppm) levels in aqueous sample. The best models for mineral prediction were developed based on the spectral variables selected by variable importance on projection (VIP) on standard normal variate (SNV) or multiplicative scatter correction (MSC) pretreated data. The best model performance for Mg revealed the R^2CV values of 0.90 and 0.91 with the RMSECV values of 0.187 ppm and 0.182 ppm, R^2P values of 0.79 and 0.77 with the RMSP values of 0.279 ppm and 0.287 ppm for the measurement temperatures of 22 ºC and 50 ºC respectively. The best models for the prediction of Ca yielded the R^2CVs of 0.85 and 0.86 with the RMSECVs of 2.522 ppm and 2.438 ppm, R^2Ps of 0.69 and 0.67 with the RMSEPs of 3.227 ppm and 3.351 ppm for the measurement temperatures of 22 ºC and 50 ºC respectively. Only cross-validation was carried out for Zn prediction, the best prediction performance revealed the R^2CVs of 0.81 and 0.76 with the RMSEVs of 0.074 ppm and 0.084 ppm for the measurement temperatures of 22 ºC and 50 ºC respectively. In this study, the GMS system combined with chemometric analysis demonstrates some potential for mineral determination in aqueous INF samples. For a future study, concentrated aqueous INF samples will be employed (e.g. 10-50%w/w) to the further exploration on the potential of GMS for prediction of other mineral elements (e.g. Fe, Cu, Na, K).

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Clémentine M. G. Charoux, BSE, M, PhD

Project Title: Design and development of novel technologies to improve the removal of biofilms and destruction of spores

Clémentine M. G. Charoux, Colm P. O'Donnell and Brijesh K. Tiwari

Project Leader: Dr. Amalia Scannell

Abstract

The microbial inactivation effects of contact ultrasound systems have been investigated in many studies. However these systems are restricted to food applications in liquid food or food immersed in liquid media. Airborne acoustic technology employing non-contact transducers is a potential technology to reduce microbial loads in dried ingredients with limited impacts on food quality. In this study, black pepper grains (*Piper nigrum L.*) and tapioca starch (*Manihot esculenta*) were inoculated with *Bacillus subtilis* vegetative cells and spores and subjected to airborne acoustic waves at 170 W for selected treatment times ranging from 0 to 150 min at room temperature. In order to assess if this technology had any significant impacts on the food quality of either dried ingredient, the total phenolic content of black pepper grains and the rheological properties of tapioca starch were assessed. Significant reductions of 2.75 log CFU/g and 2.01 log CFU/g were achieved after 30 min of treatment for tapioca starch and black pepper respectively. No significant observations in terms of food quality were noticed among treated and untreated samples. Airborne ultrasonic technology could be a potential tool for food decontamination with limited impacts on food quality.

Selected Recent Publications

Charoux, C. M., O'Donnell, C. P., & Tiwari, B. K. (2017). Ultrasound Processing and Food Quality. In Ultrasound: Advances for Food Processing and Preservation, (pp. 215-235): Elsevier.

Charoux, C. M., Ojha, K. S., O'Donnell, C. P., Cardoni, A., & Tiwari, B. K. (2017). Applications of airborne ultrasonic technology in the food industry. Journal of Food Engineering, 208, 28-36.

INVESTIGATING THE EFFECT OF PREHEAT TEMPERATURE AND SOLVENT TYPE ON DISSOLUTION PROPERTIES OF WHEY PROTEIN CONCENTRATE USING FBRM

X. Wang and C. O'Donnell

UCD School of Biosystems and Food Engineering, University College Dublin, Belfield, Dublin 4, Ireland.

Abstract

This study investigated the effect of preheat temperature and solvent type on WPC dissolution using focused beam reflectance measurement (FBRM). Higher preheat temperature affected the dissolution properties of WPC samples by decreasing the mean chord length (MCL). Dissolution of WPC was improved when dissolving in skim milk compared to in water.

Introduction

Dissolution of dried dairy ingredients, e.g. whey protein concentrate (WPC) is a time consuming process and significantly influenced by several parameters, such as protein and mineral content, dissolution process and storage conditions of powder samples (Koh et al., 2014, McCarthy et al., 2014) Evaporation preheat treatment, concentration and spray drying temperatures affect the solubility of milk powders (Oldfield et al., 2005, Kelly et al., 2002). To date, only one study by Sikand et al. (2012) was reported to investigate the effect of solvent type (water and ultrafiltered skim milk permeate) on the solubility of milk protein concentrate (MPC). Mean solubility index and percent soluble solids of MPC solution was increased, while mean particle sizes decreased when MPC was reconstituted in skim milk permeate. Skim milk permeate contains mineral salts, especially more potassium and sodium salt besides lactose and non-protein nitrogen, which enhance the solubility of MPC (Sikand et al., 2012). **The objective of this study was to investigate effect of preheat treatment and solvent type on dairy ingredients dissolution using FBRM technology.**

Materials & methods

WPC powders with 4 different preheat treatments, namely control, 72 ºC, 95 ºC and 115 ºC were studied for the dissolution properties in two solvent types, namely deionized water and skim milk. WPC powders were manufactured in a pilot scale processing facility in Teagasc (Moorepark, Cork, Ireland). Skim milk was purchased from a local supermarket (Dublin, Ireland).

Approximately 3.6 g WPC powder samples were reconstituted in 300 ml preheated solvent to achieve a 1.5% WPC powder solution at 50℃ in a 500 mL glass jacketed vessel with a recirculating chiller fitted for temperature control. An overhead 4-blade impeller was used with a rotating rate at 400 rpm. FBRM (model D600L, by Mettler Toledo) was placed in the vessel to monitor the dissolution process. The data from FBRM were collected by iC FBRM

program (Mettler Toledo), with the collecting interval set at 10 s for 30 min duration.

Three replicates were analysed on each condition to give an experimental design of 3 replicates x 2 solvent types x 4 WPC powders (n = 24).

Results and discussion

Characterisation of WPC dissolution

Fig. 1 shows changes in FBRM median chord length (MCL) during WPC dissolution in deionized water and skim milk. An initial large decrease in MCL (in the first 30 - 60 s) followed by a small increase until the end of the dissolution test was observed when dissolved in water (Fig. 1A). The initial decrease observed is caused by the powder pouring onto the water surface (Fang et al., 2010). Changes in FBRM chord length distribution (CLD) during water dissolution are shown in Fig. 2 (WPC control). During the WPC dissolution process, large particles are broken down or dissolved to form smaller particles. Because of the inherent detection limit of the FBRM, particles with chord lengths < 1 µm are not detected. Meanwhile, some of the particles may agglomerate and form larger particles (Fang et al., 2010). An increase in MCL followed by a large decrease is observed for WPC dissolved in skim milk, which can be caused by the powder pouring onto the water surface. CLDs for 30, 60, 120, 300, 600 and 1200 s are very similar for WPC dissolution in skim milk (data not shown).

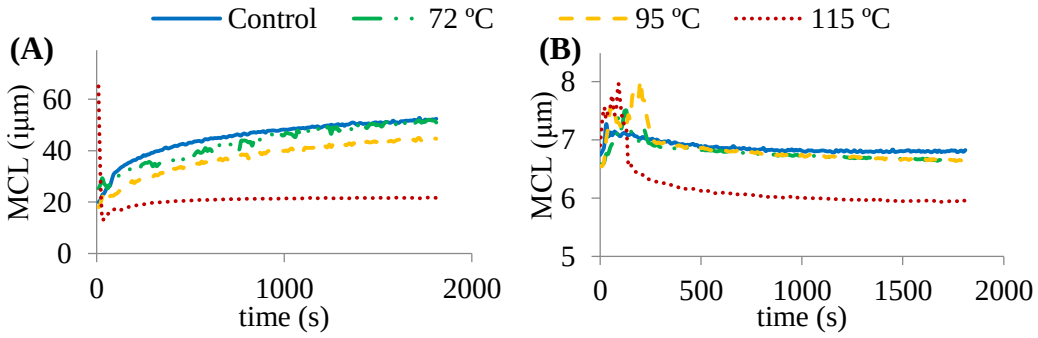

Figure 1: FBRM MCL during WPC dissolution in water (A) and skim milk (B)

Effect of preheat temperature

Fig. 3 and Table 1 show the FBRM CLD and MCL of WPC powders dissolved in either water and skim milk after 30 min. MCL decreases with the increasing preheat temperature when WPC is dissolved in both solvent types (Table 1). The CLD profiles for control, 72 and 95 ºC preheated WPC dissolved in water are similar (Fig. 3A). While CLD for 115 ºC preheated WPC has a much larger proportion of particles between 3 and 20 µm when WPC is dissolved in water, leading to a lower MCL compared to other WPC samples. CLDs for WPC dissolution in skim milk are similar and overlapped (Fig. 3B).

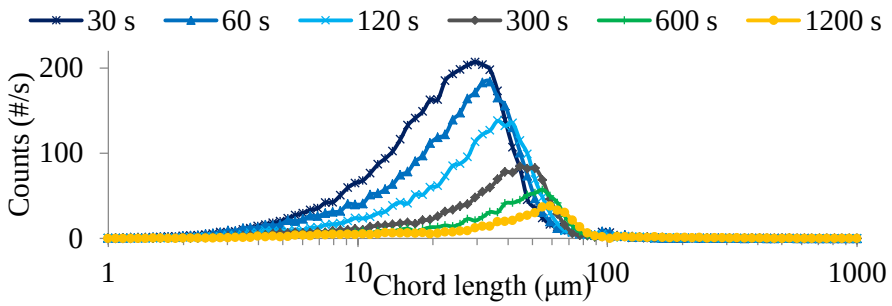

Figure 2: FBRM CLD during WPC dissolution in water (WPC control)

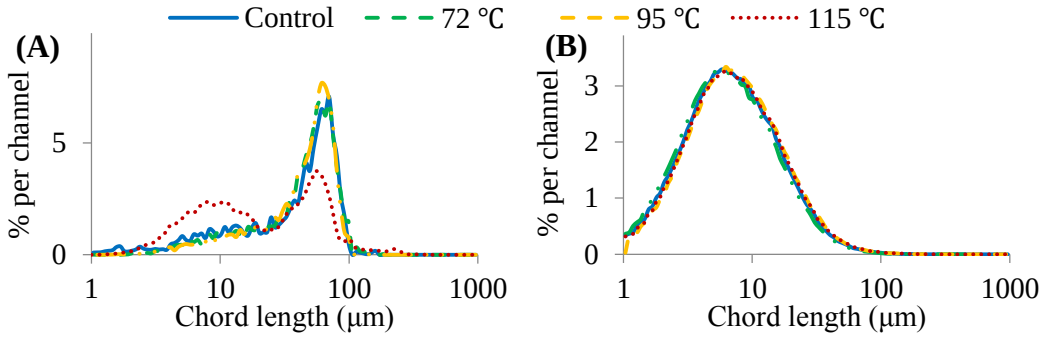

Figure 3: Effect of WPC preheat temperature on CLD in water (A) and skim milk (B)

Table 1: FBRM MCL of WPC dissolution in water and skim milk after 30 min

Powder	Water		Skim milk	
	Solvent	WPC + solvent	Solvent	WPC + solvent
Control	105.39±1.01	54.05±0.39	6.60±0.06	6.83±0.12
72 °C	106.22±1.21	51.65±3.11	6.57±0.11	6.65±0.15
95 °C	105.31±1.13	44.73±4.24	6.64±0.06	6.65±0.21
115 °C	106.11±1.17	21.72±9.96	6.60±0.08	5.96±1.28

Effect of solvent type

All WPC samples have similar profiles of MCL change with time and only result of WPC control is presented (Fig. 4). It is not possible to characterise the effect of solvent type by comparing the final MCL or CLD, while it is possible to study MCL change over time. MCL takes shorter time to reach plateau when WPC is reconstituted in skim milk, indicating dissolution is faster in skim milk then in water.

Conclusion

FBRM was demonstrated to be a potential process analytical technology (PAT) tool that can provide real time and *in situ* particle counting and sizing data during WPC dissolution processes. FBRM MCL decreased at higher preheat temperatures, due to the inherent detection limit of the FBRM to detect chord lengths < 1 µm. The use of skim milk as solvent

improved WPC dissolution.

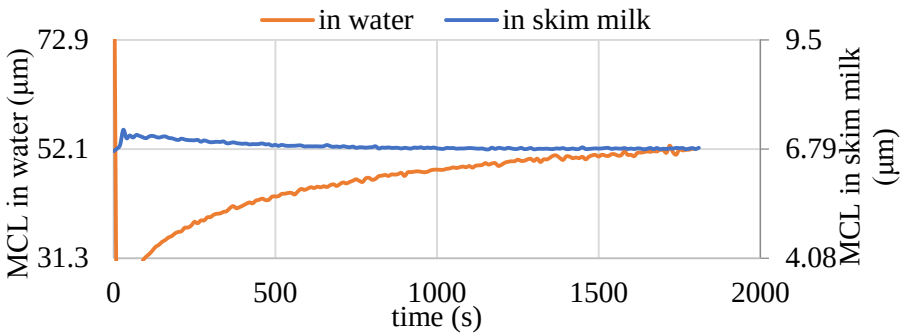

Figure 4: MCL change with time of WPC control

Acknowledgements

This work was supported by the Irish Department of Agriculture, Food and the Marine through its Food Institutional Research Measure (FIRM) (Project Reference No: 11/F/052). Xiao Wang wishes to acknowledge the Chinese Scholarship Council for financially supporting his PhD study.

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AMALGAMATION OF WAVE-PV ENERGY SYSTEMS: A FEASIBILITY STUDY ON THE IRISH SEA

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Abstract

Hybrid Renewable Energy Systems with energy storage holds great potential to deal with the unpredictable nature of renewable energy sources (RES). Currently, the major challenge with RES is their dependency on environmental conditions. E.g.: Solar Irradiance. The individual RES cannot provide continuous power supply to the load. Hence, combining multiple RES would be more reliable and environment friendly solution. The aim of this study is to determine the feasibility of integrating two sources of renewable energy, solar and wave along with energy storage system using a location on the Irish Sea. This proposed system has potential to play a key role for Ireland due to its favourable geographic location and coastline. The modelling and technical analysis would be conducted on HOMER energy modelling optimization software. Based on the potential recoverable energy production calculated, the complimentary features between solar and wave would be investigated and compared to the power demand.

Introduction

With the variable nature of renewable energy sources, a major challenge for single resource systems is the intermittent power supply and increased capital cost of power storage and management systems(Yucaosotonacuk *et al.*, 2017). To improve this energy supply stability, this paper considers use of a hybrid system that combines multiple sources together along with a system for energy storage. This hybrid system is a promising source of delivering clean energy and holds good potential considering the European Union's energy target of achieving 20% electricity from RES by 2020. The two renewable energy source considered for this study are Solar Photovoltaic and Wave energy. Solar energy is quite unpredictable, less efficient and also sunlight is not available throughout the year. Wave energy is unsuitable in extreme weather conditions and also varies within time-scales. Hence, the idea is to utilize both these RES in a way that both can rectify the faults of each other and as a whole provide uninterrupted power supply. It is estimated that between 7 to 8% of the power produced is lost through the electricity transmission and distribution system (EirGrid 2016). Hence, to reduce this, an energy storage device like a battery would be utilized for storing the excess energy produced from the hybrid system and to supply this energy to the grid in case of power shortage.

A hybrid system is defined as the combination of two or more renewable/non-renewable energy sources. The basic components of the hybrid system includes energy sources (AC/DC), AC/DC power electronic converters and loads (Krishna and Kumar 2015).This study will be focussing on the performance of 0.4 kW Solar panel and 0.55 kW wave power converter installed offshore at the Irish Sea Coast (53.8° North and 4.4° West).

The objective of this study is to determine the feasibility of integrating two types of renewable energy sources, storing the excess energy produced in a battery and identifying if the proposed hybrid system can maintain the balance between demand and supply.

Materials and Methods

Data accumulation

This paper will consider datasets for solar irradiance from The Irish Meteorological Service online (www.met.ie) and datasets of wave from Ireland Ocean Energy Expertise (www.oceanenergyireland.ie). At the same time factors such as no. of modules, maximum rated power, maximum voltage and maximum current will be considered while inputting data for solar energy system. Similarly, parameters like wave chamber length, water surface area inside the chamber, turbine inlet area and water depth will be considered while inputting data for wave energy system.

Hybrid System Assessment

To find the complimentary features of solar and wave renewable (recoverable) energy resources, a statistical correlation will be made using the Kendall Tau rank correlation. Kendall τ can then be defined and calculated as;

τ = C-D / C+D, where

C is the number of concordant pairs and D is the number of discordant pairs.

Kendall τ, a number between -1 to 1, shows how similar or different the two datasets are. A negative value means two renewable resources are likely to be complimentary to each other. (Yucaosotonacuk *et al.* 2017)

Modelling and analysis

Energy system models will be built using the energy system modelling software, HOMER. Through modelling, electricity load will be created to reflect the average energy demand and then meeting this demand shall be modelled by utilizing the hybrid energy system.
Input information to HOMER includes: electrical load data (1 year of load data), renewable resources data, component technical details(PV,hydro,battery and converter), controls etc. HOMER will then perform hundreds or thousands of hourly simulations over and over to ensure the best possible match between demand and supply to design the optimum system. Similar simulation performed for PV-Wind hybrid system by (Energy 2017)

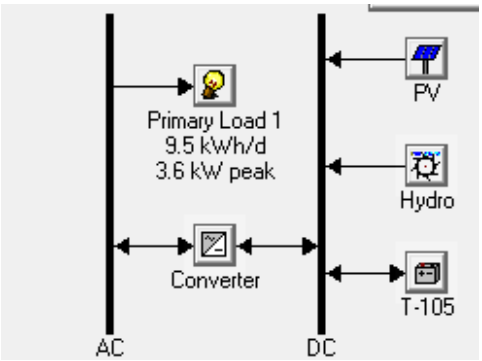

Figure 1: Schematic of Wave- PV hybrid system at the Irish Sea

Results and Discussion

Complementarity

The aim of an hybrid system is to harvest multiple renewable resources for improving the energy supply stability. As shown in Fig 1, solar energy has lower energy during winter months. Wave energy could compensate for such temporal variation during winter since it has high energy density during winter.(Yucaosotonacuk et al. 2017)

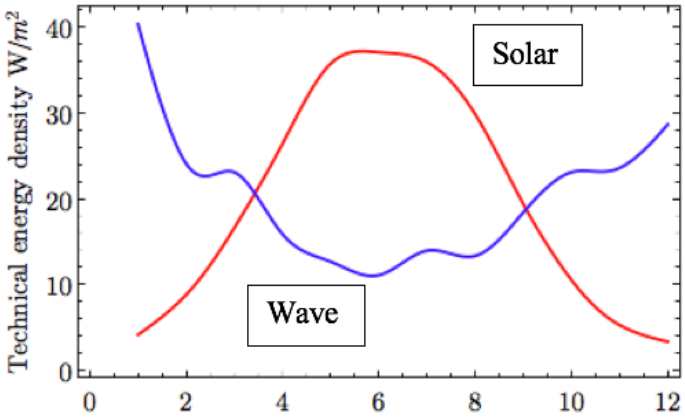

Figure 2: Monthly average technical density(Yucaosotonacuk *et al*., 2017).

Expected Results

The main aim of the proposed hybrid system is to establish an offshore commercial scale Wave-PV hybrid power plant on the Irish Sea by eliminating the nature of power generation of both wave and PV energy sources. According to a similar study conducted on the Malaysian Island, the below power distribution curves were obtained.(Fig 2)

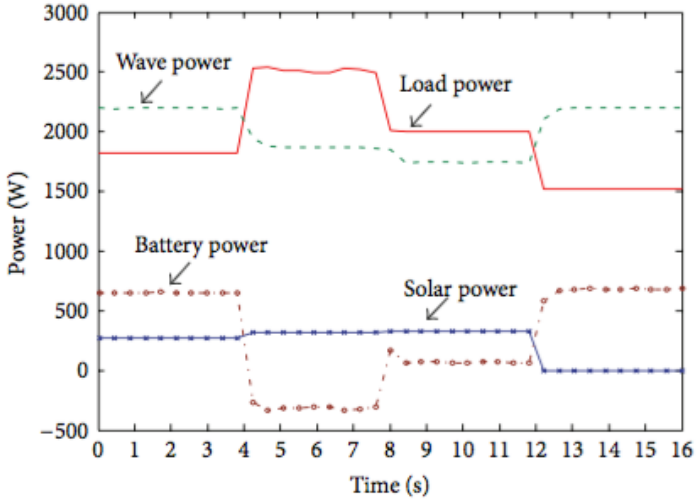

Figure 3: Wave-PV hybrid system power distribution*(Ahmad et al. 2014).*

The controller plays an important role here since it has to be developed in such a way that it can accumulate the excess power generated by the hybrid system and supply to the load in case of power shortage. It can be seen that during the solar and wave power generation and the load variations, the battery bank charges or discharges accordingly to maintain the power stability of

the whole system. Hence, it is clear that when the generated power from solar and wave is more than the load demand, the battery bank gets charged and when the load demand is more than the combined power generated, the battery gets discharged.

Conclusions

Electricity in Ireland has high CO2 emissions per kWh due to the supply mix on the national grid and high cost of electricity, along with high carbon emissions and reliance on imported fuels (CODEMA 2016.) For this reason, this study will examine the feasibility of the proposed hybrid system. After accumulation of solar and wave data for the chosen location, assessment of complementarity of both the renewable energy sources would be positive. Thereafter modelling of this system on HOMER software, the results will determine if the performance of 0.4 kW Solar photovoltaic system and 0.55 kW wave power system would be satisfactory under the steady-state as well as transient power condition thereby maintaining the balance between demand and supply.

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A FEASIBILITY STUDY FOR APPLICATION OF IRELAND'S WASTE RECYCLING STRATEGIES IN CHINA

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Abstract

This paper introduces the background of waste management China and its significant change stated in July 2017 that China enhanced the regulation regarding to the import of waste from other countries and regions. Aiming the new issues happened in China waste management system due to the restriction of importing waste, the study primary adopts Dublin and Chongqing where is a direct-controlled municipality located in southwest of China as the analysis cases to study for what extent that the Ireland's waste recycling strategies are suitable to apply in Chongqing, China. Four aspects feasibilities are undertook and compared between Dublin and Chongqing.

Introduction

China as the dominant market and the manufacturer of waste recycling made a significant change in July 2017 for regulation of importing 'foreign waste'. Chinese government states in World Trade Organization (WTO) July 18th that China will ban the import of waste from foreign in order to match the developing schedule and protect public health and environment (Toloken 2017). For more than 20 years in the past, China was so important for importing and digesting recyclable waste that, currently, the Chinese restriction of importing waste is being widely discussed in order to figure out the solution for mountainous waste.

According to the statistics of Institute of Scrap Recycling Industries (ISRI) for 2016, the United States (US) exported total value of $17.9 millions of scrap, 13.2 millions tonnes of recyclable paper and fibre, and 775,500 tonnes of plastic to China (Boteler 2018). The significant number of waste exported formed a solid industry chain provided a huge number of jobs. ISRI President Robin Wiener responded China's statement immediately in July 18th 2017 that the US industries' export activities, including waste export, supported more than 155,000 direct jobs so that it would be catastrophic result once implementing the restriction for importing waste (Carpenter 2017). Turning to Europe, majority of countries depend on the support of China for exporting waste. As for plastic waste only, China totally imported 7.3 million tonnes of it from UK, EU, US and Japan (Cole 2017).

However, the significant change on the origin of recyclable waste also intensively shocked Chinese domestic waste recyclable market, which compelled Chinese government to modify the existed waste recyclable system. Delvoie and Plessis-Fraissar indicated early in 2005 that the annual solid waste quality was predicted to further increase by 150% in 2030, namely increasing from 190 million tonnes in 2004 to 480 million tonnes in 2030. In the past decades, Chinese government had significant improved the waste management strategy (Delvoie and Plessis-Fraissar 2005) through stating new policies and laws, and learning management from developed countries. Therefore, the study mainly analyse the application of Ireland's waste recycling strategy in China.

The objective of this feasibility study was to systematically analyse whether the application of Ireland's waste recycling strategies is suitable in China and helpful for forming an efficient waste management in order to the improvement of environment.

Materials and methods

Analysing location selection

The thesis adopts Dublin and Chongqing where is a direct-controlled municipality located in southwest of China as the objects to discuss. The problem of waste management is mainly figure out how effectively deal with municipal waste so the study primary focus on the city area. According to the statistics of Central Statistics Office (2016), Dublin as the capital of Ireland has 1.3 million people lived in range of 115 km^2 and 3,677 persons per km^2 of average population density in the city area. On the other hand, Chongqing as a megacity embraces over 30 million people for the whole city, including urban and rural area, and 367 persons per square kilometres of population density (Knoema, 2015). Based on the statistics of Country Digest (2016), the population of Chongqing is respectively 8.5 million in the city proper, 18.4 million in the wider urban area and 30.1 for the municipal area. Cox (2014) in a report published on Newgeography indicated that Chongqing's urban area (890 km^2) just occupied 1/100th of whole province area. However, 3 times of population compared with national average, namely around 7,700 persons per km^2, live in the city central. Moreover, the enhanced urbanlisation and re-opened two-child policy of China caused that the population density increased to approximately 9,600 persons per km^2.

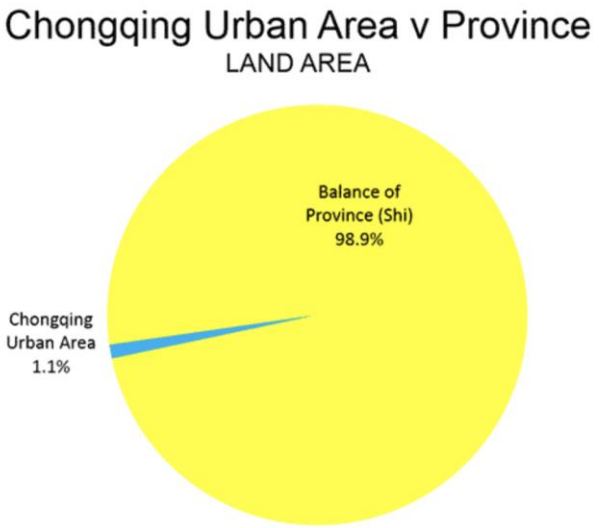

Figure 1: A comparison of land area between urban area and province in Chongqing

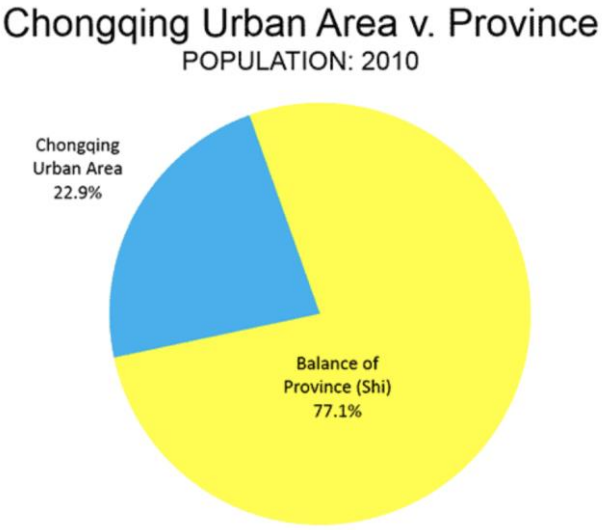

Figure 2: A comparison of population between urban area and province in Chongqing

Methods
The study will mainly adopt comparison method to comprehensively discuss the advantages and disadvantages from technical feasibility, economic feasibility, policy feasibility and society feasibility.

As for the technical feasibility analysis, the study will compare the development of technology between Ireland's and China's, including current situation and future potential. The efficiency of each technology will be also compared in order to support the results. Furthermore, the improvement of waste technology demands the support of economy and policy, and the consensus of society as well. Aiming to the economy and policy aspects, the detailed and up-to-date government reports can be quoted to as the references. In addition, those that has been applied similar strategies and its consequences are useful as reference group. Finally, the society feasibility study depends on the latest public opinion researches for waste management on the society.

In addition, the study will focus on waste plastic recycling strategies due to the recent change on the restriction of importing waste from foreign published by Chinese government. Although the waste management is a thorny issue in a long term and has been improved on some aspects awing to the effect of China, the unemployed persons caused by the statement of restriction and the following a series of issues mightily shocked the current waste management systems and markets in China. It must be admitted that the application of importing waste restriction increased the possibility of applying the Ireland's more integrated waste recycling strategies.

Results

According to the adopted methods for the feasibility study, there are several expected results. Firstly, the most ideal consequence is that all the results indicate that Ireland's waste recycling strategies are suitable for applying in China be it for technology, economy, policy responses or social consensus. Secondly, the outdated technology of waste management system results in fail to apply. Thirdly, it is high possibility to fail because of the inconformity of social consensus that is caused by the difference on public opinion between Ireland and China.

Discussion and conclusion

As for the expected results, the reasons of causing the results would be analysed and discussed. Whatever applying the strategies in Chongqing is feasible or not, the reasons would be studied. The significant change leading by China aiming to the importing waste policy is increasing its impact for global waste trade market. The responded new strategies are demanded for all the influenced countries and regions, especially Europe and the United States. The study focused on technology, economy, policy and society aspects is a opportunities to answer how to improve the efficiency of waste management for China so that reduce environmental pollution and solve the problem caused by the restriction for importing waste. In a nutshell, the study method design demands improvement to enhance the reliability of the results, but the ultimately results are potential for implementing the waste management and providing opportunities for responding the new waste recycling environment in China.

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FEASIBILITY COMPARISON OF FORESTRY VS BEEF/SHEEP FARMING VS GROWING GRASS FOR BIOGAS PLANTS IN THE NORTHWEST OF IRELAND

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Abstract

Profits in beef and sheep farming are minimal in the Northwest of Ireland, averaging between 13,000 and 16,000 euro per year. Alternative solutions are available such as forestry and growing grass for potential biogas plants. Grass is an excellent energy crop due to long persistence of high yields accompanied by low energy inputs. The most important factor for the successful development of biogas production from grassland is the knowledge of the specific yield of biogas (methane) and the potential of the biomass and methane yields per hectare. Forestry is a market which is demonstrating a high return value per acre, although is not particularly well received by small enterprise beef and sheep farmers in the Northwest. The introduction of improved tariffs is necessary if the 'Green Energy' industry in Ireland is to flourish in the future.

Introduction

The agricultural sector in the northwest of Ireland is a demanding and shifting sector. Much of the poorer quality land is now moving towards forestation, which is predominately not well received in many areas. Leitrim, West Cavan, Donegal, Sligo and North Mayo are areas which are worst affected by afforestation. Forestry is becoming a tempting option for many farmers due to the lack of financial security linked with much of farming practices in operation. These include sheep, suckler and beef farming enterprises, while dairy farming on average is the most profitable by nearly 200% (Donnelly, 2015). Reduced interest or take of farming by young people can be observed due to the lack of financial profit linked with farming in the Northwest of Ireland.

Anaerobic digestion (AD) is the process of decomposition of organic matter by a microbial consortium in an oxygen-free environment (B.F. Pain, 1985), into biogas and digestate. Biogas plants can be feed with a wide range of feedstocks from agricultural residue (slurry/grass/silage), Domestic and food processing waste and crops grown specifically for AD (Wholecrop wheat/maize). A rich mixture of feedstocks is inserted into a sealed airless container and the contents will be heated to accelerate the process, where bacteria will decompose the material and produce biogas (Caslin, 2016). Biogas can then be used to generate heat or electricity or both through combined heat and power (CHP) is the most common. All power outputs can be used on site of production for own consumption or either supplied to the grid.

The objective of this study is to determine the feasibility of growing grass for biogas production in the northwest of Ireland, as an alternative to forestry and beef/sheep farming.

The future for AD in Ireland is a prosperous one. Farming in the Northwest of Ireland is challenging, and many see it changing into an area which is predominately unwanted, forestry. The potential for farms to grow grass for biogas production is more favourable option for farmers who wish not to go down the forestry line or are choosing of changing their

enterprise direction. However, is the financial and feasibility present in Biogas production to allow farmers with an alternative.

Materials and Methods

Potential of grass silage

Grass is a readily available resource in Ireland, which we must make full value of. Compared with other feedstocks, grass has suitable and promising characteristics as energy crop for biogas production. Because of its assurance on availability of throughout year and conservation, ensilage or haylage are indisputable, (Konrad Kocha, 2009). Perennial grasses, especially are excellent feedstocks for renewable energy production in support of several rationales such as high potential of dry matter yields, fast growth, and additional potential use of inputs compared to annual crops.

Data analysis

In this study, any values which cannot be found for the Northwest of Ireland or each individual county, the national average will be used.

Results and Discussion

Farmers profits

Half of farmers located in the northwest of Ireland who carried out the survey would be interested in supplying grass to a Biogas plant. 65% of the farmers interested would do so for the 'better financial incentive' and security which a contract with the Biogas plant would offer, while the rest of the votes were split evenly to 'produce power for on farm use' or 'To produce power and sell it to the national grid'. Of the 65% of the farmers surveyed two-thirds were either beef or sheep farmers, who on average demonstrate a 75% more reliance on direct payments towards incomes (Emma Dillon, 2017). Dairy farmers, who made up the final one-third of the farmers surveyed, maintain approximately €40,000 income per annum over beef and sheep farmers. As a result, it can be assumed the increased averaged income is the reasoning why dairy farmers have less of an interest in supply grass to a Biogas plant. Table 1 below illustrates the average farming income per farming practice.

Table 1. Average Farm Income 2016 and Average Farm Income by Farming Practice 2017

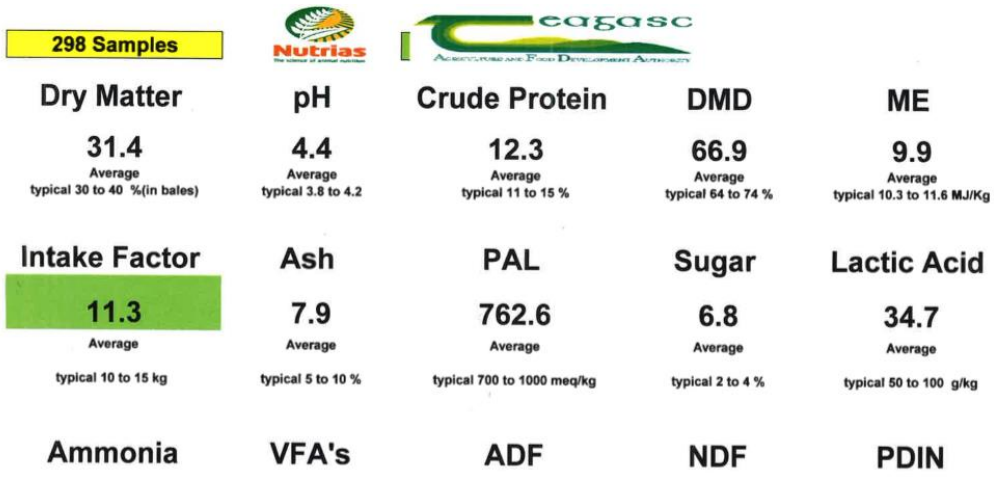
County	**Average Farm Income 2016 €**	**Farming Enterprise**	**2017 Average Farm Income by Farming Practice €**
Cavan	19,257	*Dairy*	52,000
Leitirmx	10,671	*Sheep*	16,000
Sligo	12,064	*Cattle Rearing*	13,000
Donegal	12,209	*Cattle Other*	16,500
Mayo	11,208	*Tillage*	34,000
Monaghan	21,900		

Source: (Teagasc, 2017)

Table 1 above outlines the average yearly income for each county in the Northwest of Ireland. 2016 illustrates an average farm income of €24,060, all the counties in question are below the national average. Some counties are not even half the national average.

Grass quality

298 grass samples were sent into Aurivo this spring. Majority of the samples received are in the Northwest and West of Ireland. Samples consisted of grass silage which were cut in the summer of 2017. Grass silage with a dry matter (DM) of 25% will produce on average 151m3N biogas /t, (Kennedy, 2010), making it a viable and abundant alternative feedstock. 31.4% was the average DM of nearly 300 samples of silage from the 2017 yield. Though grass silage may be less energetically productive when compared to maize silage, it still offers a good energy balance and environmental advantages (Gerin PA, 2008). Grass can be an excellent energy crop and may be classified as a high yielding (up to 15 t dry matter ha).



Forestry

The government's national strategic plan for forestry in Ireland is to expand from 11% to 18% of the land area by 2046, in a bid to offset carbon emissions, (Cormack, 2018). The most recently available statistics indicate that Co. Leitrim has the second highest acreage of forestry at 16.7%, just behind Co. Wicklow at almost 18%. Leitrim, Cavan, Mayo, Roscommon and Sligo – have seen a significant increase in planting, accounting for one third of the afforestation programme in 2016, (Cormack, 2018). Sitka Spruce is the most common species of tree planted in Irish forestry, accounting for approximately 60%. Sitka Spruce grows well in Ireland because it is suited to our soils and climate. Planting Sitka Spruce provides financial incentives of €440/ha for the first 15 years of the plantation lifespan. Farmers are also able to retain their single farm payments while having planted forestry on their land, which is a huge financial bonus.

Conclusion

Grassland is the dominant agricultural landscape in Ireland, covering 91% of the 4.3 million hectares of agricultural land. The size of the national herd has decreased and will continue to do so in the future. The potential to produce grass silage for biogas production is increasing annually if the financial security is present. Diversification of agricultural enterprise to grass biomethane production will assist rural development through sustainable employment, security of energy supply, and environmental benefits associated with reduced stocking rates. The financial incentives which forestry provides are very hard to match, hence why farmers in the Northwest are moving into that sector and away from cattle and sheep farming. However, producing grass silage for biogas production is an option which must be installed more in the future in the likes of the Northwest of Ireland. Currently, Ireland is paying 12c for biogas €per kw, which is 6c below the average of Europe. The finances in operating a biogas plant in Ireland currently isn't feasible unless the government offers increased tariffs for biogas production. Until then, it is unlikely that we will see many more biogas plants been erected in Ireland.

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THE UTILISATION OF INDOOR FARMING TO REDUCE IRELAND'S OVER-RELIANCE ON THE COW

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Abstract
Humankind is entering an era of unprecedented change that is already affecting and will continue to affect the global food supply. Dramatic change is coming caused by overpopulation with an increased demand for more food together with global warming. Rearing and grazing livestock is a notorious resource-inefficient method of farming and due to the nature of Ireland's reliance on animal production, it must import most of its food from other nations in order to sustain itself. This study theorises the potential to revolutionise the current agri-food system by employing new age farming technologies and techniques. These methods can potentially help fight food insecurity and climate change thus securing a sustainable food supply for future generations. EU legislation regarding new farming systems and the feasibility of implementing indoor/urban farms within Irish cities using existing infrastructure to mitigate environmental impact of such establishments will also be investigated.

Introduction
There are currently 7.6 billion people on the planet. Each and every person should have a fundamental right to access food to support themselves, yet this is not the case. It is estimated that over 2 billion people suffer from the 'hidden hunger' of micronutrient deficiencies (Godfray et al, 2014). Furthermore, the amount of people estimated to be on the planet by 2050 is around 10 billion, which is an almost 50% increase in population in a little over 30 years (United Nations, 2017). In addition, global warming is causing the weather to become increasingly volatile. Climate change is causing fluctuations in rainfall patterns, warmer temperatures which can dry out soils and cause drought and other frequent extreme weather conditions (Wheeler et al, 2013). It has never been more essential for a nation to have a self-sufficient supply of food.

Ireland, although it is seen as an agricultural leader by other countries due to its 'green' image has been a net importer of food since the early 2000's (AgriLand, 2016). This country is a leader in dairy and beef production, but because of this, the country relies massively on other nations to feed itself. 81% of Ireland's agricultural land area is devoted to pasture, hay and grass silage (3.63 million hectares) to be fed to the nation's livestock sector (mostly cattle), 11% to rough grazing for said livestock (0.47 million hectares) and a mere 8% to crop production (0.38 million hectares). Beef and dairy alone account for over 68% of the country's Gross Agricultural Output (DAFM, 2014). Most of the available arable land is connected in some way to cattle, either for tillage or grazing and so there is not much available land remaining to expand the nation's crop production by conventional farming methods as these require large areas of land. In light of these facts, this paper will examine the feasibility of proposing an alternative to this inefficient resource-intensive farming culture through the utilisation of indoor farming systems.

The objective of this study is to showcase how modern indoor farming techniques can be utilised in Ireland to expand the scope of the agri-food industry to cater for more crop production, thus reducing the country's reliance on livestock to keep the industry afloat and the reliance on other nations in order to feed its people.

Materials and Methods

In order to fully appreciate the possible benefits and negatives of utilising indoor farming technologies on a large scale within the Irish food industry, there are some key areas that must be considered in this study. These areas will be researched and inspected with extreme detail to highlight the possible strengths and flaws regarding the implementation of indoor/urban farming practices.

Threats

There are a few major issues affecting global and national food security today. Increased pressure on the demand for more food as a result of overpopulation and an increased overall per capita consumption coupled with the ever-increasing unstable weather conditions that come with climate change are all factors straining food security worldwide (Godfray et al, 2014). The very way humans grow and consume food is changing landscapes and societies worldwide. Relying on other countries to feed our population does not make logical sense in this rising food insecure state the world is currently in. It is now vital, more so than ever, in human history to reduce waste in food production and consumption and utilise less resource intensive farming techniques all while producing a better yield of food. This has come to be known as 'sustainable intensification'. This is a more sustainable means of cultivation environmentally coupled with intensifying the production of food growth. This paper will examine the threats that are currently affecting and will affect global and national food security highlighting why it is necessary to revolutionise the current farming model that is overwhelmingly susceptible to these changes.

Conventional Farming vs Indoor Farming

There are a couple of major issues that traditional farming models are subject to which can have detrimental effects on crop yield. Due to the nature of growing crops in soil outdoors on a vast array of land, there are many variables that can affect the quality and security of a farmer's harvest. It is estimated that 20-25% of harvested crops worldwide are lost due to pre and post-harvest diseases, pests and climatic changes and this is only going to increase in the future (Dixon, 2012). In times of increased food instability within the world, these inefficiencies simply cannot be afforded. Indoor farming is the idea that instead of growing food horizontally outdoors subjecting crops to a host of variables that can damage the harvest while using a vast array of land in the process, we should instead grow produce vertically indoors. Growing crops indoors enables the farmer to cater for every aspect of a plants growth cycle such as light from artificial lighting and recycling water in a closed loop system via the use of hydroponic or aeroponic systems. These systems spray the roots of crops with water and a nutrient mix solution providing all the necessary conditions to induce photosynthesis while eradicating the need for growth in a soil medium so as to not contribute to any more soil degradation and using far less water in the process. Because these farming systems are indoors the crops are not subject to changes in weather conditions, pests or disease like traditionally grown produce is. Indoor farms are carefully controlled environments with the hope to grow more with fewer resources (Chance et al, 2017). Conventional farming vs indoor farming is a serious debate that is taking place in many corners of the globe today and this study will seek to address the positives and negatives on both sides of the spectrum by simply looking at the facts and statistics both farming systems have to offer and ultimately come to a conclusion on the superior farming system pertaining to specific crop types to be grown in Ireland.

Light

Understanding how light affects and induces plant growth is a vital factor in understanding indoor farming systems. Light can be expressed as a wave and the size of the waves (wavelengths) can vary depending on where the wavelengths fall on the electromagnetic spectrum. The spectrums wavelengths can be measured in units known as nanometres (nm) and range from 0 to 5,000,000,000 nanometres. However, the light visible to human beings only falls between a tiny fraction of this spectrum between 400 to 700 nm. Every single colour that is known to humankind falls in between a

small section of the overall spectrum, but it is here that the spectra of light have the most impact on plant growth (Vadiveloo et al, 2017).

Light emitting diodes (LED's) have gained a significant amount of attention with indoor and would-be indoor farmers due to their potential as a single or supplemental source lighting system for crop production both terrestrially and extra-terrestrially. The challenge, however, is determining an optimal design for the plant lighting system in order to calculate the exact wavelengths essential for specific crop types. This is a challenge because the output waveband of LEDs is a lot narrower than conventional sources of lighting that have been used for plant growth in the past. In spite of the challenge of perfecting the design of this lighting system their potential over traditional light sources is evident as their operational lifetime and durability is significantly higher, their small size makes them easy to manoeuver and re-calibrate, their ability to change the wavelength specificity output and their cool emitting surface makes them the ideal evolutionary successor to previous light sources (Massa et al, 2008).
This paper will attempt to create an index which showcases the favourable spectra of light that are required by indoor farms utilising LED's in order to induce optimal growth performance in the top crops consumed by the Irish people to investigate the feasibility of growing these crops in country.

EU Policy
Investigating current EU laws and regulations regarding the establishment and implementation of indoor farming systems in order to create a possible new network of farms within Ireland is essential to the validity of this study. Perhaps EU law prohibits the creation of new farming systems as it could hamper an already established food chain within the European Union and its member states despite how inefficient this may be. Perhaps there are no incentives or subsidized grants to indoor farms, therefore, rendering the possibility of establishing this practice in Ireland null and void. However, it is known that the European Union has developed support policies to increase the production of environmentally friendly organic food (Nikolic et al, 2017). Due to the nature of indoor farming practices, no pesticides or herbicides are needed in order to grow crops. As a consequence of this, indoor farming produce can be categorised as organic and the EU's current legislation on this practice could be the perfect incentive to establish this farming system. Examining all aspects of EU law is vital to ensuring a successful creation of a new agri-food industry within Ireland that can bring stability to its over-reliance on cattle and ultimately lead to job creation and food security for its people.

Feasibility and Implementation
This paper has a few specified primary objectives. However, the utilisation of Ireland's 'Emerald Isle' image in order to establish itself as an agricultural leader with indoor/vertical farming technology is perhaps the main objective. The methods of farming that are already used by established companies and countries alike will be investigated thoroughly to examine whether this technology can be harnessed and set up in Ireland to the benefit of its people. Surveys will also be conducted with members of the Irish public in order to understand their overall knowledge of where their food comes from and to gain a better understanding as to whether they would choose to support this possible future farming model.

The specific location of an indoor farm is vital to its success. Reducing the distance between grower and consumer is a top priority within the urban farming ethos and due to this farming systems mantra, available rooftop space that is yet to be harnessed around cities like Dublin via office buildings, apartment blocks and schools will be investigated to examine the feasibility of setting up these high-tech farms throughout the city. A timeline for future endeavours will be speculated, calculated and drawn up in order to envision a highly functioning network of indoor/vertical/urban farms throughout Ireland. This could potentially sustain the population with home-grown healthy local produce going

into the future while mitigating the effects of global warming and sharing some of the burdens the livestock industry carries with the current agri-food system established in the country.

Results and Discussion

It is a very early stage in the research of this paper and so there is no clear result with regard to the theory put forth by this thesis. The theory of whether utilising indoor farming systems can be used to reduce Ireland's over-reliance on the cow will remain unanswered until all categories within the materials and methods section are thoroughly investigated. However, the expected results of this study are that, with the implementation of indoor/urban farming systems within Ireland, will indeed feasibly be implemented to establish the Irish food sector as an agricultural leader. Thus sustaining the people on locally grown produce instead of being a net importer of food and aspire to become a net exporter of food while reducing the need to rely so heavily on cattle in order for the agri-food industry to stay afloat.

Conclusion

Through the creation of a ‘light index' for LED induced crop growth this thesis aims to be a one-stop shop regarding the exact spectra of light needed to induce efficient and economical crop growth with Ireland's most popular foods. The establishment of a hypothetical network of future indoor farms and the creation of a timeline to set up this network through a feasibility study aims to establish a viable plan regarding the establishment and implementation of indoor/urban farming practises utilising modern technologies within Ireland. If all areas of research within this paper are carried out effectively it can only expand the consciousness of the Irish people to realise that although overpopulation and climate change may seem like daunting concepts for the future of food security, there is also a great opportunity afoot to mitigate the effects of both factors which could be capitalised upon with the right information and farming methods.

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FEASIBILITY OF PUMPED HYDROELECTRIC ENERGY STORAGE IN IRELAND AT BOTH MICRO AND CONVENTIONAL SCALE

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Abstract

Ireland is one of many countries seeking a viable solution for the problems relating to renewably sourced energy intermittency and variability. Bulk energy storage is seen to be the most promising solution and of the various bulk energy storage technologies available pumped hydroelectric energy storage is by far the most well established. In this study the feasibility of a large scale pumped hydroelectric energy storage (PHES) facility and a network of sub-micro PHES units at multiple sites in Ireland are assessed and compared based on set criteria and HOMER software analysis. The expected results find that the large scale PHES is the more viable of the two options though a network of sub-micro PHES units may one day be feasible through further study and investment.

Introduction

Countries around the world are currently striving to decarbonise energy systems in an effort to prevent further dangerous climate change and improve overall sustainability. There has been widespread development of variable renewable energy generation technologies and a corresponding increase in bulk energy storage systems research (Barbour *et al* 2016). One bulk energy storage system that has seen a renewal of interest is PHES. In terms of energy security Ireland is very vulnerable as it lacks indigenous fossil energy resources and therefore must rely heavily on importing fossil fuel from abroad. This puts Ireland in a politically, geopolitically and geographically vulnerable position (Goodbody *et al* 2013). As of 2016 the contribution of renewables to Irelands gross final energy consumption was only 9.5% (SEAI 2017) even though there are enough indigenous renewable resources available to supply all the required energy (Connolly *et al* 2011). In the face of climate change and given Irelands vulnerability it is essential Ireland utilises its renewable resources more effectively both to ensure its energy security, and to avoid hefty fines for not meeting the relevant EU renewable energy targets. One of Ireland's greatest resources is wind however, like many other forms of renewable energy, wind energy suffers from intermittency and dispatchability issues (Zhao *et al* 2015). Bulk energy storage systems are needed to solve this issue and improve the penetration of renewable energies such as wind energy. PHES is the most mature and commercially-acceptable bulk energy storage technologies available (Rehman *et al* 2014). Numerous studies have shown PHES to be a viable bulk energy storage option for use in conjunction with renewable energy sources (Zhao *et al* 2015; Coburn *et al* 2014).

There is currently only one PHES plant in operation in Ireland known as Turlough Hill which is owned by the ESB and has a energy storage capacity of X. New PHES projects being considered in Ireland include the Knocknagreenan (70MW), Kippagh Lough (70MW) and Glinsk (1200MW, seawater plant) plants (Geth *et al* 2015). This study builds on the work of previous studies to assess the feasibility of PHES in Ireland. As well as assessing the feasibility of more traditional large scale (>30MW) plants this study will also assess the feasibility of a network of micro scale (<100KW) PHES units.

The objective of this study is to assess and compare the feasibility of both large scale pumped hydroelectric energy storage facilities and a network of micro scale pumped hydroelectric energy storage units in Ireland.

Materials & Methods

This study will predominantly take the form of a theoretical study with some minor use of energy systems modelling software for more detailed modelling analysis. The methodology outlined below represents basic framework this study will follow but may be subject to change over the course of the study.

Site selection
First the identification of suitable sites in Ireland for both the large scale PHES facility scenario and a network of micro PHES units scenario will be undertaken. For the more traditional large scale facility any possible site must have the following basic the criteria; the presence of a high head, suitable topography, geological impermeability, geotechnical conditions, access to the electricity transmission network and water availability (Coburn et al 2014). It is important to note that both freshwater PHES and seawater PHES will be included in this.

In the case of the network of micro PHES units however a slightly different set of criteria will be used in the selection of a suitable site. Taken inspiration from using individual car batteries as a way of storing energy the micro PHES units would be built into either new or existing buildings to form a network type bulk energy storage system. A suitable site or community for the network of micro PHES units will share some similarities with the large scale PHES facility such as the presence of a high head for each unit and water availability however, the head height will be determined by the height of the building and the water availability will be determined by the available space for two separate water reservoir tanks. Grey water could be used in this scenario Other criteria will include: the number and type of buildings.

The above information will be gathered from previous studies done, and publicly available sources such as the Ordinance Survey of Ireland. Figure 1 below provides a basic illustration

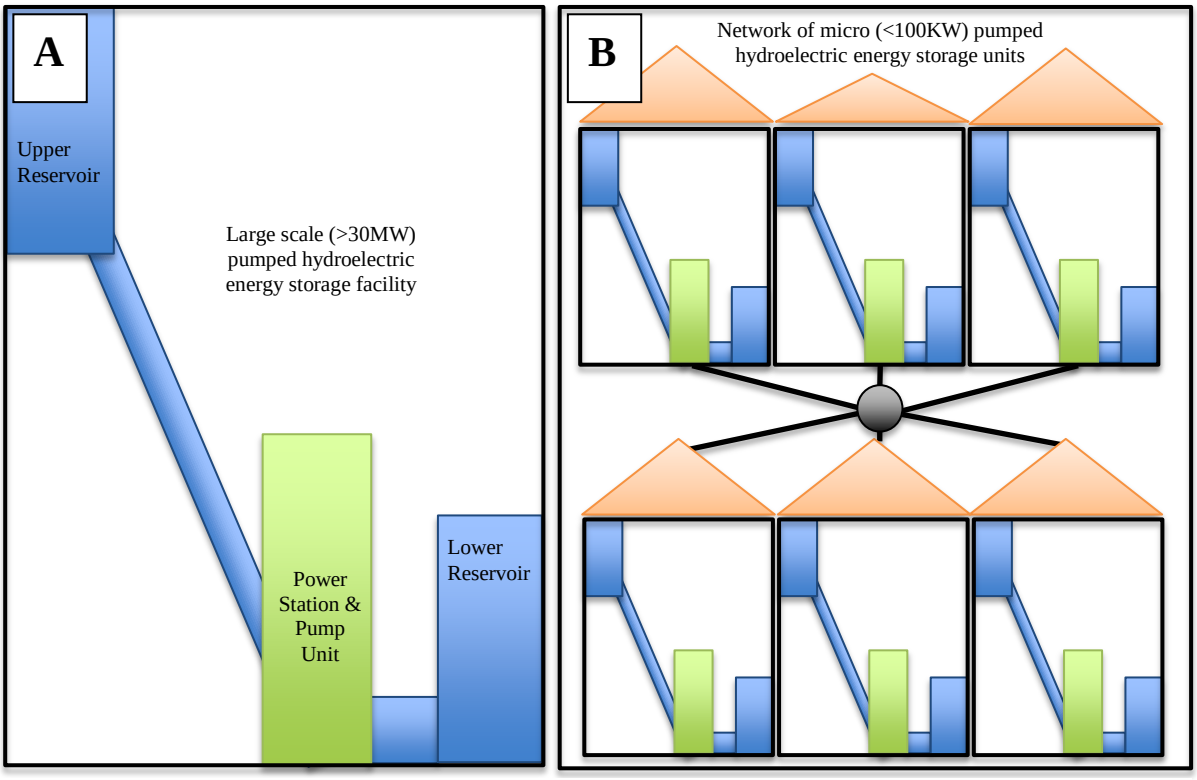

Figure 1. (A) A basic illustration of a traditional PHES facility. (B) a conceptualized basic illustration of a network of mirco PHES units with multiple bulidings all connected to a centralised control hub (the black circle).

of the two scenarios to be assessed in this study.

PHES Feasibility Assessment
Upon the selection of suitable sites for both of the two possible scenarios each chosen site will undergo further assessment looking at the feasibility of using the PHES technology there. This will take the form of a technological-economic-environmental assessment. The energy storage capacity, capital cost, operation and maintenance cost, land use change, and environmental impact will be assessed.

HOMER Analysis
Some modelling and analysis may be conducted using HOMER (Hybrid Optimization of Multiple Energy Resources) energy systems modelling software. This will be done to aid in identifying suitable sites for each of the two scenarios being assessed. Once the sites have been identified further size optimization and sensitivity analysis of the considers systems will be performed (Bhatt et al 2016).

Comparison
The optimum configurations chosen from the results of the feasibility assessment and HOMER analysis for both the large scale PHES facility scenario and the network of micro PHES units will finally be compared to determine which of the two is the most feasible option is. The selection of the optimum configurations will be based on the lowest net present cost (NPC) and cost of energy (COE) as well the minimum associated environmental impact.

Results and Discussion

As this study is still in its early stage of development there are no formal results as of yet. What follows is a brief discussion of the expected results to come based on preliminary research into the current literature.

Expected Results
It is expected that a number of acceptable sites will be identified, particularly along the west coast of Ireland, for large scale PHES facilities. Of these possible sites it is most likely that less than half will ultimately be viable options following the feasibility assessment. Previous studies have found that suitable sites often reside in nature conservation zones, and in remote areas which are lacking in energy demand (Coburn et al 2014). Nevertheless, a small number of feasible sites are expected to be found.

In the case of a network of micro PHES units it is believed that any suitable sites that are found will be in areas of high urban density. Issues that may arise with the feasibility include the efficiency of the PHES unit, the structural dilemmas with regard to the installation of the PHES unit and with economies of scale (Oliveira, Hendrick 2016).

Future Work
Firstly, an extensive literature will be carried out building on the current body of work presented here. From this the methodology will be further developed, improved upon and extended in greater detail. The data required for this study shall be gathered and analysed subject to the outlined methodology ultimately providing the final results for a detailed discussion and final conclusion.

Conclusions

Based on the expected results it is concluded that the more traditional large scale PHES facility will most likely be determined the most feasible of the two scenarios in Ireland however it is expected that with further study and investment the application of micro PHES technology may one day become a feasible option.

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EVALUATING THE OPTIMUM LOW TEMPERATURE DISTRICT HEATING NETWORK DESIGN FOR AN IRISH APARTMENT BLOCK BASED ON THERMAL LOAD ANALYSIS

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Abstract

Low temperature district heating networks utilise renewable and waste heat sources to provide low-carbon thermal energy to end users. Despite successful implementation in other countries, and the clear environmental benefits, there are very few district heating networks installed in Ireland. This project aims to design a cost effective, low temperature district heating network for a new Irish apartment block. To achieve this, thermal load data of Irish apartments will be obtained through measurement and building simulation modelling with Energy Plus software. This data will then be used to perform a thermo-economic analysis of a low temperature district heating network, designed for an Irish apartment block. This analysis will determine the most cost-effective network configuration for an Irish apartment block. It will determine factors such as the optimum supply & return temperatures, heat exchanger size, pump size and network flow rate that result in the shortest return on investment for the network.

Introduction

In recent years, efforts have been made to reduce Ireland's dependence on fossil fuels in the heating sector. District heating (DH) can reduce emissions in this sector but has been underutilised in Ireland to date. District heating is an efficient method of supplying low carbon thermal energy to buildings. It is a system in which heat is produced centrally by one or more energy sources and then transported through a network of pipes to an end user (European Commission 2016). Fourth generation district heating (4GDH) is the latest generation of heat network design. 4GDH operates at lower supply temperatures than previous generations and in doing so allows waste heat sources to supply networks. 4GDH can also integrate renewable heat sources such as solar and geothermal heat (Lund *et al.* 2014; Ziemele *et al.* 2017). DH offers many environmental benefits with almost half of energy in the Danish DH networks coming from renewable sources (Buhler *et al.* 2017). Despite the clear benefits of district heating, Ireland has the second smallest installed capacity in the EU (Andrews *et al.* 2012).

District heating networks must meet the thermal demand of the end user at all times. An important factor in the design of DH networks is therefore the estimation of network peak thermal load. Overestimation of thermal load results in peak load boilers being oversized. This results in unnecessary capital costs and lower operating efficiencies. Estimating peak loads also enables network pipe capacity to be correctly sized which creates savings and reduces distribution losses (Li and Wang 2015). Furthermore, thermal load data can also help identify viable opportunities for thermal storage on DH networks that reduce demand peaks and operating costs (Gadd and Werner 2013a). The thermal demand of buildings depends not only on physical factors such as weather, but also social factors such as the requirement for hot water in the mornings. Both of these factors vary from country to country (COHEAT LTD 2014). In Ireland, opportunities may lie for DH implementation alongside newly constructed apartments however a lack of information exists regarding thermal load profiles of Irish occupants. If this information were available, it would enable cost effective and efficient DH networks to be designed. There is clearly scope for the study of thermal load analysis of Irish residential dwellings, constructed to post 2016 building standards.

The objective of this study is to calculate the thermal load profiles of Irish apartments and hence perform a thermo-economic analysis of a low temperature district heating network, designed for an Irish apartment block built after 2016.

Materials and Methods

Thermal load data

As mentioned, the thermal load profile of a dwelling depends not only on physical factors such as weather but also social factors. Different types of occupants, such as families, students, or pensioners, have varying heat demand preferences. To build a realistic representation of an apartment block's thermal load profile, data must be available for various occupant types. Data relating to the thermal load demand of students will be obtained from the University College Dublin (UCD) Cyclon Active Energy Manager database (Cyclon 2018). Thermal load data relating to other occupant types has been requested from Dublin City Council, but this has not yet been obtained. If sufficient thermal load data cannot be obtained, then occupancy profiles, available in literature, will be utilised through Energy Plus software to calculate thermal load profiles (Kane *et al.* 2015).

Building energy modelling

Energy Simulation Modelling software, such as Energy Plus, can be used to estimate building thermal load profiles (Cho *et al.* 2013). If measured thermal load data cannot be gathered, an energy simulation model of an Irish apartment will be created. Such a model will require weather data, occupancy data and building thermal envelope data. The output from this model will be an hourly thermal energy demand profile of a new Irish Apartment for each month throughout the year. Occupancy data for different socio-economic tenant types will be input into the model to determine respective load profiles for each occupant type. By combining these individual load profiles, the load profile for an entire apartment block that represents the demands of different occupant types, will be obtained (Buhler *et al.* 2017). Irish weather data will be obtained from the Energy Plus weather database. It is hoped that building envelope data of a recently built apartment will be obtained from Dublin City Council or UCD. Occupancy data, representative to different socio-economic groups is available in literature ,(Kane *et al.* 2015).

Apartment block district heating design

The apartment thermal load profile obtained will then be used to design a low temperature district heating (LTDH) network for an entire Irish apartment block, built to recent building standards. This will be a thermo-economic analysis that determines the optimum DH network supply temperature, return temperature, pipe size, heat exchanger size and pump size that can meet the thermal demands of occupants while minimizing lifetime cost. There are many trade-offs that exist in designing such a network. For instance, as supply temperature decreases, network efficiency increases however the size of cost of heat exchanger and network pump then also increase which leads to a rise in capital cost. This model will determine the most cost-effective network configuration.

This study will apply the same approach to that of Park et al (Park *et al.* 2017). Here, domestic hot water and space heating loads were obtained using TRNSYS software. This data was then used to carry out a LTDH thermo-economic analysis of a 15-story apartment block in Korea. A supply temperature of 60°C was calculated to give the shortest payback period for the network. The apartment block modelled in this project will likely be smaller than this example as apartment blocks of this size are not common in Ireland. This analysis will be carried out using MATLAB software.

Expected Results

Thermal load profiles

Hourly thermal load profiles of an Irish apartment at different months throughout the year will be obtained for varying occupancy types. This will enable the thermal load of an entire Irish apartment block to be estimated. An example of a typical apartment load profile can be seen in figure 1 below.

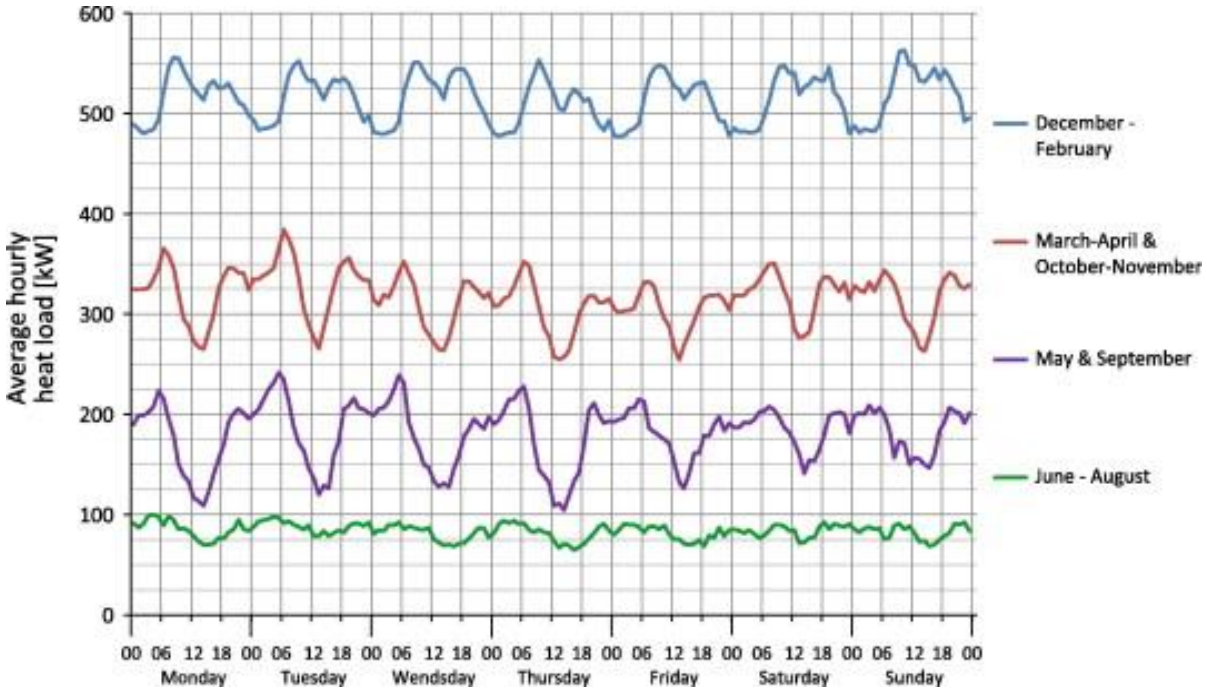

Figure 1: The average weekly heat load patterns of a Swedish apartment block across four seasons (Gadd and Werner 2013b).

As can be seen from figure 1, the thermal load varies throughout the day due to social factors but also varies seasonally due to climate. A similar result to this data will be expected in this project.

Thermo-Economic analysis
The thermo-economic analysis of an Irish Apartment LTDH design will calculate the optimum supply and return temperature network. It will also determine the pipe, heat exchanger, and pump sizing that will ensure the shortest payback period.

Conclusion

Upon the successful completion of this project, a model will be created that can determine the optimum LTDH network design for a newly constructed Irish apartment block. This model will use measured thermal load data where possible and data from a building simulation model when this is not possible. The socio-economic background of occupants significantly effects thermal load profile. This model will incorporate thermal load data from various occupant types to create a model representative of Irish heat demands.

If Ireland is to reduce its reliance on fossil fuels to supply thermal energy, then district heating must be embraced. The model developed in this study will be of use to planners and developers who wish to install LTDH to newly built apartments. The thermal load data that will be compiled will also be useful in the design and sizing of Irish DH networks.

Acknowledgements

The author acknowledges Donna Gartland at Codema for her guidance to date in the area of district heating in Ireland.

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PHOTOVOLTAICS IN INDIA - A FEASIBILITY STUDY

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Abstract

Solar energy is the fastest growing renewable energy source in the world. Power output from a PV module is influenced by a number of parameters. Ambient temperature is an essential parameter that decides the power output from a PV module. The variation of power with temperature is an intrinsic property of the base material and there are wide variations to the extent to which power output is affected by changes in temperature. Parametric calculations indicate that this variation is minimal for PV modules based on amorphous silicon and highest for PV modules based on crystalline silicon wafers. It is identified that amorphous silicon based PV modules are best suited for the warmer climate present in South India.

Introduction

An ever growing demand for energy coupled with the depletion of the existing fossil fuel resources and a pressing need to combat climate change have been the significant factors that led to the research in the field of renewable technologies and solar energy in particular (Goura 2015).

India has an abundance of solar energy due to its close proximity to the equator. The country, on average, receives 3000 hours of sunshine per year which is equivalent to 5000 trillion kWh which is thousands of times greater than the total energy consumed per year (Sudhakar *et al* 2013). India has set ambitious targets to install 100 GW of photovoltaics by the end of the year 2022 under the Jawaharlal Nehru National Solar Mission (JNNSM) plan. (Ministry of new and renewable energy 2015), hence it is worthwhile to look at how effective photovoltaics would be in India.

The power output from a solar cell depends on a variety of climatic factors of the location where it is installed and also on the type of material and design type used to make the solar cell. The most significant of these would be the ambient temperature and hours of direct irradiance (Chander *et al* 2015).

The ambient temperature is a function of the latitude of a location and India being a country with a large latitude variation in latitude of about 30° (8°N at Kanyakumari to 38°N at Kashmir) there are large variations in temperature extremes as the latitude increases and relatively lower variations at lower latitudes, also the average annual temperatures also decrease with an increase in latitude (Revadekar *et al* 2012), hence there is a large variation in temperatures across India.

To measure the effect that the variation of ambient temperature has on the efficiency of a solar photovoltaic modules made of different materials and to identify which material is best suited for each geographic location considered.

Materials and methods

Data collection

Solar irradiance data was taken on a 15 minute intervals for all 5 geographical locations under consideration (Kochi, Ahmedaad, Delhi, Kolkata, and Nagpur). Data for ambient

temperatures were collected for similar intervals and interpolated to obtain a self-consistent set of values.

The values for the temperature and irradiation coefficients are given below (Table 1).

Table 1. β_{ref} and γ values for different materials (Virtuani *et al* 2010)

TCO's	Pmax γ_{rel} (%/°C)	Voc β_{rel} (%/°C)	Isc α_{rel} (%/°C)	FF κ_{rel} (%/°C)
Error	**± 0.027**	±0.021	±0.019	-
a-Si (SJ)	**-0.13**	-0.33	+ 0.12	+ 0.10
CdTe	**-0.21**	-0.24	+ 0.04	- 0.01
Microm. (a-Si/μcSi)	**-0.36**	-0.37	+ 0.05	- 0.04
CIGS	**-0.36**	-0.31	+ 0.02	- 0.08
c-Si wafer-based	**-0.45**	-0.33	+ 0.06	- 0.19
TF - Si	**-0.48**	-0.41	+ 0.15	- 0.22

Data analysis and calculations

The power output from a photovoltaic module is given by the equation,

$$P_{out} = I * \eta_c * A_{PV},$$

Where, P_{out} is the power output from the module, η_c is the efficiency of the module, and A_{PV} is the area of the module.

The temperature dependence of the module efficiency is governed by the equation,

$$\eta_c = \eta_{Tref}(1 - \beta ref\,(T_c - T_{ref}) + \gamma \log 10\,(I\,(t)))$$

Where,

$$T_c = T_a + (T_{NOCT} - 20) * (I\,(t) / I\,(t)_{NOCT})$$

Here, η_{Tref} is the efficiency of the module at the reference temperature, β_{ref} is the temperature coefficient of the material used, T_c is the cell temperature, T_{ref} is the reference temperature, γ is the solar irradiation coefficient of the material used, I (t) is the solar irradiance as a function of time, T_a is the ambient temperature, and T_{NOCT} and I $(t)_{NOCT}$ (open circuit condition measurements) are intrinsic values for the different materials (Dubey *et al* 2012).

The materials considered in this study are amorphous silicon, multi-crystalline silicon, and CdTe. All factors other than intensity of incident radiation and ambient temperature are kept at standard test conditions so as to facilitate a fair comparison between the different technologies.

Analysis of the results obtained are carried out using a spreadsheet software and graphs are used for this purpose

Results

Correlation of ambient temperature and power output

The variation of the power output from the different materials used for making solar cells as a function of temperature is given in figure 1.

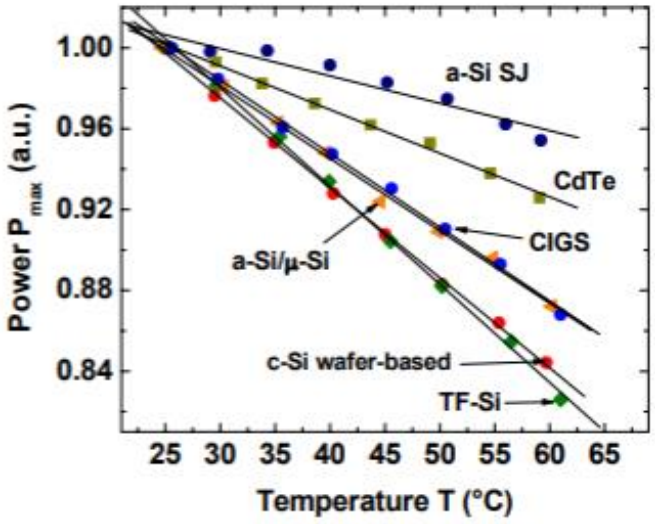

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Figure 1. Temperature-output power graph (Virtuani *et al* 2010).

As can be seen from the graph, the power output from a solar cell is directly proportional to the ambient temperature. The technology that experiences the least reduction in the power output is the amorphous silicon PV module while the one that experiences the highest reduction in power output is the crystalline silicon wafer based PV module.

Table 2. Power loss for different materials at different temperatures (Virtuani *et al* 2010).

TCO for Pmax γ_{rel}, (%/C)	This work	Internal database (SUPSI)	Manufac. Datasheets + Literature
a-Si	**-0.13 (SJ)**	-0.1 to -0.3 (SJ, DJ, TJ)	-0.1 to - 0.3 (SJ, DJ, TJ)
CdTe	**-0.21**	-0.2 to -0.22	-0.18 to -0.36
Microm. (a-Si/µc-Si)	**-0.36**	-0.26 to -0.38	-0.24 to -0.29
CIGS	**-0.36**	-0.26 to -0.36	-0.33 to -0.5
c-Si wafer-based	**-0.45**	-0.41 to - 0.57	-0.37 to -0.52
Thin film Si	**-0.48**	-	- 0.58 to -0.62

Table 2 shows the percentage values for power loss for the different materials that are used to make PV modules at different temperatures greater than the reference temperature (25° C) and it can be seen that the amorphous silicon based PV module is best suited for use in regions with high temperatures as it has a comparatively insignificant reduction in performance at usual ambient temperatures. South India has average annual temperatures that

are significantly higher than North India (Revadekar *et al* 2012), and hence amorphous silicon based PV modules would be more effective in such a situation.

Conclusions

The temperature dependence of the power outputs of PV modules based on different materials were calculated and the results are analysed. The material that was found to be most suited for use in regions of India with high values for average ambient temperatures (South India) was identified as amorphous silicon.

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GOAL & SCOPE OF A COMPARATIVE LCA ON THE ENVIRONMENTAL IMPACTS OF A WASTE HEAT DISTRICT HEATING SYSTEM TO SERVE SOUTH DUBLIN COUNTY COUNCIL BUILDINGS.

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Abstract

With time running out to reach GHG and renewable energy targets, the need for renewable heating in Ireland has grown. 4th generation district heating can utilise low temperature heat sources like waste industrial heat, giving it the potential to replace traditional heating system in urban areas. South Dublin County Council plan to build a large-scale district heating utilising the waste heat from Tallaght's Amazon data centre to heat its municipal buildings. To decide if this system is the optimum in terms of fossil fuel depletion and GHG emissions an LCA will be conducted using Gabi. The proposed systems are the waste heat system, a biomass CHP plant supported by individual gas boiler and an individual gas boiler only system. The LCA will encompass the raw material acquisition, plant construction, use phase, decommissioning and waste disposal.

Introduction

Ireland is facing a binding EU 2020 target to reduce greenhouse gas (GHG) emissions by 20%. EU Renewable Energy Directive (2009/28/EC) committed Ireland to produce 16% of all energy consumed from renewable sources by 2020. The 2010 National renewable energy action plan (NREAP) has set a target of 40% of electricity and 12% of heating to come from renewable sources by 2020. However, by 2016 only 6.8% of heating and cooling came from renewable sources with very little growth from the 2009 figure of 4.2% (DCCEA, 2018).

Heating & Cooling are the EU's largest energy sector making up 50% of final energy consumption in 2012. Renewables accounted for 18% of the primary energy supply for heating and cooling in 2012, while fossil fuels accounted for 75% (European Commission, 2016). However, some countries have implemented a renewable heating plan since the 1980's with 67% of Sweden's heating coming from renewable sources.

District heating is a heat distribution system where heat is generated outside in a centralised building and transferred to several buildings. It has appeared in many renewable heating plans due to its ability to integrate many different heating sources including renewables, waste heat and electric heating pumps. 4th generation district heating is identified by its ability to supply low temperature district heating to space heating and its utilisation of low temperature sources (Lund *et al 2014*). The system can distribute heat with low grid losses and can integrate a thermal grid into a smart energy system.

Traditional heating systems are individual heating systems, typically powered by fossil fuels. These systems have higher heat losses, have a greater carbon monoxide risk and leave consumer at greater risk of market volatility than district heating systems. In 2015, 71.8% of residential final energy consumption came from fossil fuels, while 25.4% came from electricity and 2.9% from renewables (Howley *et al* 2016). South Dublin Council's buildings are currently powered by individual gas boiler which are over 15 years old so are inefficient and in need of replacement.

As part of the EU Heatnet project, South Dublin County Council plan to develop Dublin's first large scale district heating system serving South Dublin Council buildings. Which consist of three separated buildings, a Library, a Theatre and an Arts Centre. The initial connection will harness the waste heat of Amazon's Tallaght Data Centre to the South Dublin Council building, so the first study system will model this connection. A Biomass Combined Heat and Power (CHP) plant to power the building has been found to be economically feasible (Gartland *et al* 2014).

The aim of this project is to set out an appropriate goal and scope for an LCA into the environmental impact of the three heating system options.

Materials and Methods

What is an LCA?

Lifecycle assessment is used to assess the environmental impact and resource depletion in a product's lifecycle from raw material acquisition to the product's end life. According to ISO 14044 standards there are four phases of an LCA: goal & scope definition, inventory analysis, impact assessment and interpretation (ISO, 2006). This paper will consist of the goal & scope of the project with expected results. An LCA goal & scope requires setting an adequate system boundary and impact categories based on the goal, which will be adhered to during the rest of the report.

The LCA will be completed using the 8.2.0.55 version of Gabi (2017) which is an LCA accounting tool. Gabi allows the user to develop a model that the user can add designed processes using data they have gathered, or they can add from Gabi's pre-existing processes list. The program will add up the data, using in- program conversion factors to provide the user with results on their chosen impact categories.

Systems

In the first system waste heat from the data centre is harnessed through an on-site energy centre by air source electrical pumps situated in the data centre's ventilation system. The electric heat pumps will heat water to 25^{o}C. This will then be transferred to an absorption heat pump station sited on a council owned brownfield site (Fig. 1) which will step up the temperature from ~25^{o}C on the secondary side to 70^{o}C on the primary side. The council building will have the existing gas boiler replaced by a Heating Interface unit (HIU) with a pump, control valves and meter situated in the pump station. The water will be pumped to the council building with the existing radiator and wet system being maintained. The total installed pipeline will be 736 metres long.

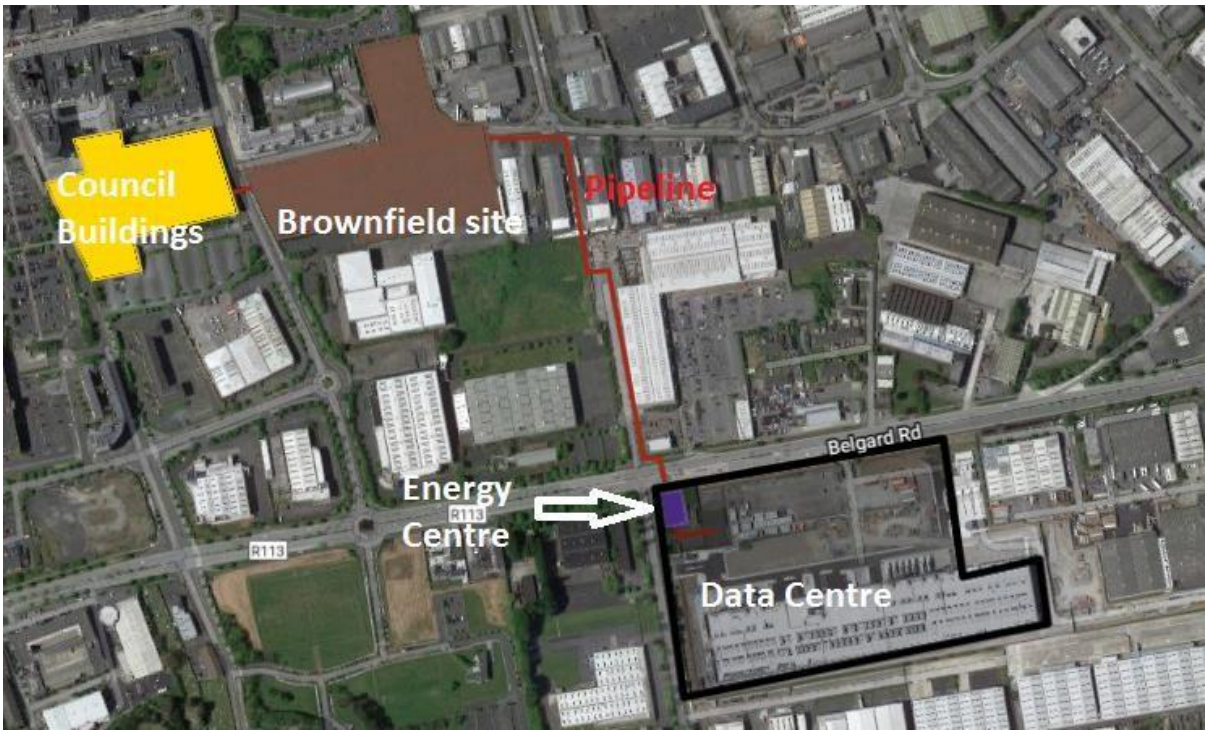

Figure 1: Proposed South Dublin County Council District heating system (Google Maps)

The second system consists of a 4MW Biomass CHP plant built on the council brownfield site to deal with the baseload with the existing gas boiler dealing with the peak demand. A feasibility study into a potential district heating system in Tallaght found this system had a payback period of 15 years (Gartland *et al* 2014). The CHP will produce temperatures of 75^{0}C and electricity will be sent

to the grid at an efficiency of 86% (54% Heat and 32% Electricity production) which is in line with the average in Irish CHP units (SEAI, 2012). The existing gas boiler will be replaced by a Heating Interface unit (HIU) with a pump, control valves and meter contained in the Council main building. A pipeline will connect the CHP to the Council building. Biomass acquisition system boundary will be based on the biomass energy generation chain in Murphy *et al*, 2014 and Murphy *et al*, 2016.

The third system consists of maintaining the existing individual gas boilers in each of the council buildings. These boilers were installed 18 years ago and the efficiency has decreased so the LCA consist of the lifecycle of replacing these boiler with new efficient gas boiler and maintaining the rest of the heating system.

System Boundary

The goal of the LCA is to analyse the GHG emissions and resource depletion of each heating system over its life cycle. The reason for the report is to find out if the assumption that waste heat would be the most environmentally beneficial option for the heating system is correct. It will help South Dublin County Council in designing plans for the district heating system.

The main function of the system is to produce heat with the production of electricity being a by – product so the functional unit will be MWh of heat. The system boundary will consist of the full lifecycle of each system starting with the retrofitting and installing of infrastructure including the acquisition of raw materials (Fig. 2). The Fuel Acquisition phase will assume waste heat of the data centre isn't assigned emissions as the data centre function is not to produce heat. However, as the biomass CHP plants main function is to produce heat, the emissions data will be included with the electricity produced assigned its share based on previously mentioned efficiencies. The gas will be assumed to be average Irish national gas mix with a connection to the gas grid already existing. The system also includes the maintenance, the decommissioning after its life expectancy and the disposal of associated process waste.

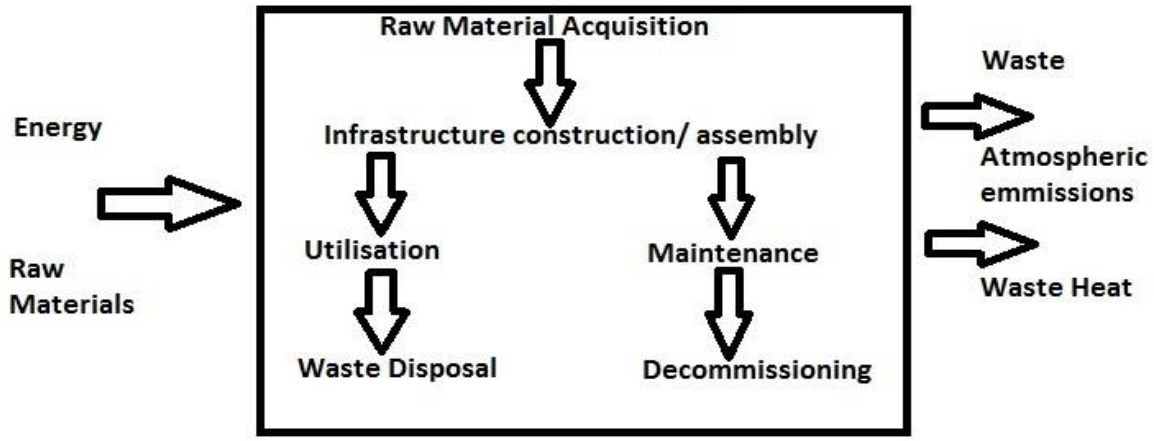

Figure 2: LCA system boundary

Impact categories

As the goal of the LCA is to analyse the GHG emissions and resource depletion, the impact categories will be global warming potential (GWP) and fossil fuel depletion (FFD). GWP is a relative measure of the heat trapped in the earth atmosphere from GHG's by assigning a relative warming potential to emissions. FFD is the sum of fossil fuels used in each system's lifecycle, with biomass being counted as renewable for this purpose.

Expected Results

In Gartland (2014) an environmental analysis was carried out on the biomass CHP plant with individual gas boiler system and the individual gas boiler only system. It found that the biomass CHP plant with individual boiler produced 9000 tonnes of CO^2 less than an individual gas boiler only system per year. However, this analysis assumed that biomass is carbon neutral which is true under EU legislation however this is not the case in LCA terms. Also, the environmental analysis only included the use phase of the heating systems. This report will provide a more accurate and in depth environmental analysis of the full lifecycle of the systems.

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FEASIBILITY STUDY OF CO_2 PLUME GEOTHERMAL SYSTEM IN GERMANY – COMBINING ENERGY GENERATION WITH CARBON CAPTURE AND STORAGE

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Abstract

To reduce greenhouse gas emissions, Directives on renewable energy usage have been set by the European Commission with the objective to reduce overall emissions by 40% by 2030 which presents a significant potential for renewable energy sources. At the same time, it is a challenge for these energy technologies which can only be solved by integrated solutions. Carbon capture and storage combined with geothermal energy could serve as a novel approach to reduce CO_2 emissions and facilitate some of the negative impacts associated with fossil fuel-based power plants as well. In the European Union Germany is the most energy intensive country with an untapped potential for geothermal energy in the northern as well as the southern regions. The CO_2 Plume Geothermal system using supercritical CO_2 as the working fluid can be utilized in natural high porosity and permeability reservoirs with temperatures as low as 65.8 °C.

Introduction

With an increasing concern about global warming incentives has been made to reduce greenhouse gas emissions. In the European Union, Directive 2012/27/EU sets target goals to reduce emissions by 20% by 2020. However, continuing progress is needed as by 2030 emission levels should be reduced by 40%. Geologic CO_2 sequestration has been considered and promoted for reducing anthropogenic CO_2 emissions from fossil fuel-based power plants that serve as a base load and balancing capacity (EC policy framework 2014). Unlike most renewable energy sources geothermal energy is a viable option in terms of consistent, reliable electricity production without the need for energy storage. In spite of this, geothermal energy represents only 3.2% among renewable sources within the European Union (Eurostat 2017). Among the member states, Germany is the biggest energy consumer while only producing half of its energy needs. Also - Germany is still highly dependent on fossil fuels like hydrocarbons and coal (Eurostat 2017). In this study a new approach to geothermal energy is investigated with the possibility of Carbon Capture and Storage, hence to serve not only as a renewable source, but to further sequester CO_2 a greenhouse gas responsible for global warming. A conventional geothermal system is connected to volcanic activity where the geothermal fluid (water) is used to extract the heat from a reservoir. Randolph & Saar (2011a) have investigated and invented a technology to utilize geothermal energy in sedimentary basins where natural high porosity and high permeability reservoirs are present. Instead of water, they modelled the use of supercritical CO_2 as the geothermal heat extraction fluid. Due to the better thermodynamic and fluid mechanical properties of CO_2 it is possible to utilize geothermal energy in areas where temperature of prospective reservoirs are as low as 65.8 °C (Randolph & Saar 2011b). The Federal Government of Germany has created an opportunity for new projects offering a feed in tariff of 25.20 cents per kWh for geothermal electricity (EEG 2017) while promotes and support the installation of renewable heat for buildings.
The goal of this study is to investigate the possibility of using the CO_2 Plume Geothermal system in Germany, to select a region with sedimentary basins and to assess the economic feasibility of energy generation and carbon sequestration.

Materials and Methods

CO_2 Plume Geothermal System (CPG)

The CPG system described here (Randolph & Saar 2011b) involves the pumping of supercritical CO_2 into natural high porosity and permeability reservoirs. The injected CO_2 is heated by the geothermal heat flux from Earth's interior. At the production side of the system the CO_2 is utilized either for electricity production through a turbine connected to a generator, or in a binary cycle through a heat exchanger to provide energy for electricity generation, and/or direct use of the thermal energy in district heating systems (Figure 1.).

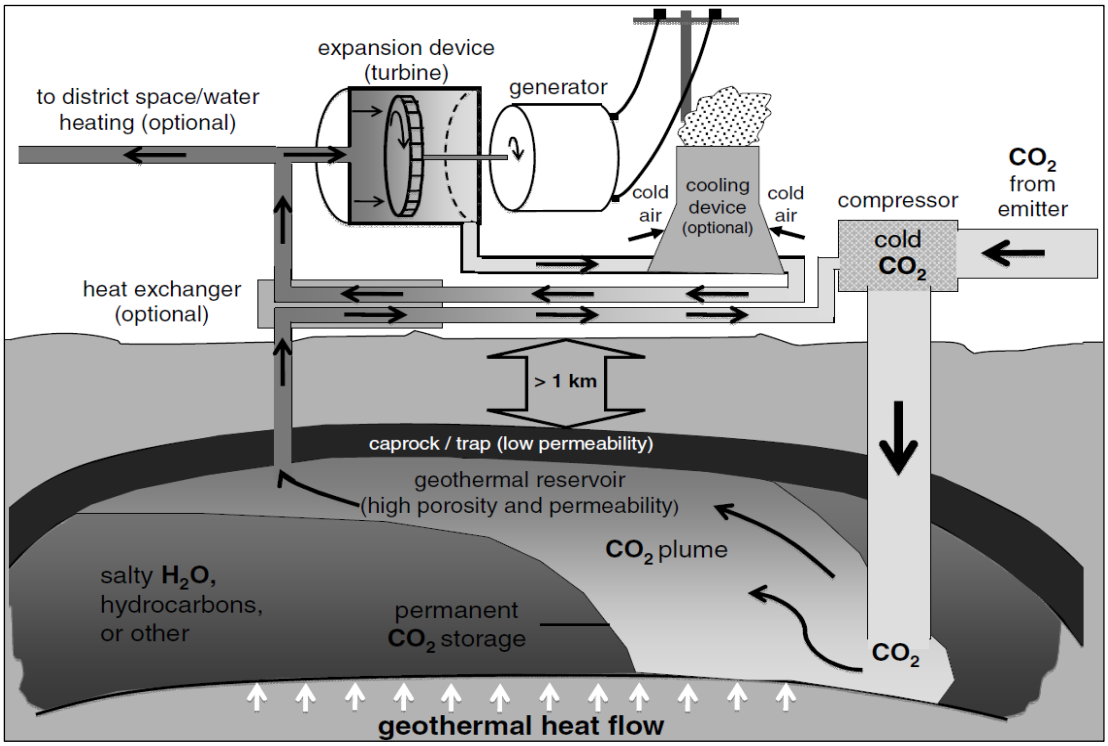

Figure 1. Schematic representation of the CO_2 Plume Geothermal (CPG) system showing the possibility of CO_2 sequestration and scenarios with optional elements for electricity production, or district heating systems (Randolph & Saar 2011b)

Determination of heat extraction rates and CO_2 Sequestration

The possibility of a geothermal system coupled with CO_2 sequestration has been investigated previously (Randolph & Saar 2011a). Those authors have determined that such a system can provide three times greater heat extraction rates compared to conventional water-based systems (Randolph & Saar 2011b). A numerical simulation is used to assess the available thermal energy. For a base case the parameters shown in Table 1. were used in a reservoir simulator TOUGH2 (Pruess, 2004) with a supplementary fluid property (CO_2, water, NaCl) module ECO2N. The model was constructed as a reference for a five-spot well configuration with 1 km^2 map view area and 707.1 m between the injection and the production wells. For the modelled scenario the heat extraction rate was calculated as 47.0 MW, averaged over a 25-year period. The issue of CO_2 sequestration is an interesting topic that can be measured in two scales. First there is the concept of traditional Carbon Capture and Storage, where the amount of sequestered CO_2 is calculated according to the occupiable space in the reservoir. Secondly a natural 5% fluid loss is expected using CO_2 as the working fluid in tight reservoirs. Randolph & Saar (2011b) are calculating this with a 7% loss based on the assumption that fluid loss is higher in naturally permeable formations. This means a permanent e.g. non-recoverable CO_2 fraction during the operation period of the power plant.

Table 1. Base case parameters for reservoir simulation

BASE CASE PARAMETERS			
Geological formation		**Injection/ production conditions**	
Thickness	305 meters	Formation map-view area	1 km^2
Well separation	707.1 meters	Temperature of injected fluid	20 °C
Permeability	$5x10^{-14}$ m^2	Injection/production rate	max. 300 kg/s (variable)
Porosity	20% (0.2)	Downhole injection pressure	26 MPa
Rock grain density	2650 kg/m^3	Downhole production pressure	24 MPa
Rock specific heat	1000 J/kg/°C	Injection/production duration	25 years
Thermal conductivity	2.1 W/m/°C		
Formation initial conditions		**Formation boundary conditions**	
Fluid in pore spaces	All CO_2	Top and sides	No fluid or heat flow
Temperature	100 °C	Bottom	Heat conduction, no fluid flow
Pressure	25 MPa		

Potential sites in Germany

In Germany geothermal electricity generation is based on binary cycle systems either as Kalina cycle, or Organic Rankine cycle. Current installations spread across the Upper Rhine Graben, the North German Basin and the South German Molasse Basin. In the North German Basin six Mesozoic sandstone aquifers exist as potential reservoirs. However, due to extensive salt tectonics a great variation in depth and thickness is recorded along short distances (Weber *et al* 2015). The Molasse Basin in southern Germany is made up by Tertiary, Upper Jurassic and Triassic sediments. The Upper Jurassic karstic limestone is a significant and one of the most important reservoir in Central Europe due to its widespread presence and high productivity (Weber *et al* 2015). The Upper Rhine Graben is a 30-40 km wide graben from Basel, Switzerland to Frankfurt, Germany. It is connected to a rift system where six potential aquifers are present for the utilization of geothermal energy. While the precipitation of minerals during production is a major obstacle especially the abundant calcite scaling in geothermal wells in the Molasse Basin, the use of CO_2 as the working fluid would eliminate the need of expensive treatment as well (Wanner *et al* 2017). In addition, Germany's widespread and strong industrial sector complement the demand for reliable renewable energy. Moreover, 55% of the final energy consumption in Germany is accounted for district heating, hot water and process heat (Weber *et al* 2015) that could be supplied by the direct use of geothermal energy.

Economic feasibility model

For the economic feasibility various software and methods are considered. The Geothermal Energy Technology Evaluation Model (GETEM) is an acknowledged tool to assess the levelized cost of electricity. Resource temperature, depth, extraction mode (binary cycle) as well as the exploration, drilling costs, field gathering and pumping, operating and maintenance and overall power plant costs are considered. The JEDI-GEOTHERMAL Jobs and Economic Development Impact Model is more complex taking into account the labour cost from exploration, drilling, field development to power plant construction and operation. It calculates with the created jobs during the project as well as all the components in the power plant (turbine, generator, heat exchanger), thus is more precise, but requires extensive research for input data. With HOMER Energy's package the possibility of integration with other renewable and non-renewable sources can be assessed either as grid connected, or as a stand-alone solution for industrial applications.

Expected Results and Discussion

The aim of the project is to locate a prospective site for the installation of the CO_2 Plume Geothermal system. Parameters for the reservoir simulation have to be researched but based on Randolph & Saar (2011b) as well as Weber et al, 2015 calculations will be performed for natural high porosity and permeability formations existing in northern and southern Germany. The support of geothermal energy is favourable in Germany as a feed-in tariff exists for a 20-year period. Moreover, the cost of drilling and construction of the power plant will be offset

by the CO_2 sequestration as an additional layer to the renewable energy generation facilitating an existing fossil fuel-based power plant as the source of CO_2 as well.

Conclusions

Although, Geothermal energy is a mature technology it is represented with the least ratio among renewable sources. This might be due to the conventional approach to geothermal energy where an adequate heat source and the presence of the geothermal fluid is required. To promote geothermal energy a new approach is recommended where emerging and novel technologies facilitate the use of geothermal energy across a broader aerial scale. Also, the hydrocarbon industry with its well-established exploration, production and development background could profit from a simple shift of a technology and move towards a more sustainable future.

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REMOTE SENSING OF SURFACE WATERS IN IRELAND

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Abstract

The EU Water Framework Directive (WFD) requires the periodic monitoring of water bodies for reporting its ecological status. One of the parameters used for calculating ecological status of water bodies is the composition, abundance and biomass of phytoplankton. The phytoplankton growth in standing waters, is traditionally indicated by the concentration of chlorophyll a. Due to the large number of lakes in Republic of Ireland (12,000), only a small proportion can be included in the National Lake Monitoring programme (2 %). Similarly, Ireland's Coastal and transitional waters are approximately 14,000 km^2 of which only 4,000 km^2 is monitored under the WFD. Remote sensing could provide cost effective solution for this problem.

Introduction

Seas around Europe are prone to the phenomenon of algal blooms, resulting from the phytoplankton growth during the spring season. However, some species of phytoplankton can form harmful algal blooms (HABs) that have the potential to kill marine creatures and cause illness in humans. In recent years, the frequency and extent of HABs has increased considerably due to pressure from human activities. Reasons for this include, the increased discharge of substances such as fertilizers from farms and, untreated waste from waste water treatment plants into the water bodies. In order to fulfill the policy objectives of EU Water Framework Directive, EU Marine Strategy Framework Directive, EU Integrated Maritime Policy and EU bathing Water Directive, it is essential to monitor and control toxic algal blooms (Copernicus.eu, 2018).

Copernicus is the European Union's Earth Observation Programme, to monitor earth, its environment and ecosystems for the ultimate benefit of all European citizens. It offers information services based on satellite Earth Observation and in situ (non-space) data. Remote sensing, in general, analyses the radiation measured by a distant sensor to derive information of a certain object such as a water body. Employing remote sensing for aquatic monitoring, could result in a cost-effective way of assessing the unmonitored water bodies as the remote sensing imagery provided by COPERNICUS is free.

By utilizing the remote sensing service offered by COPERNICUS, Ireland can capitalise on its substantial investment into the COPERNICUS programme and effectively meet its requirements under the WFD especially regarding the frequency and intensity of algal blooms, which is currently not assessed but has socio-economic and health implications. (EPA Research Call, 2017)

The goal of this research is to develop a suitable methodology to gather information on the ecological quality of the Surface waters in Ireland through the remote sensing data offered by COPERNICUS.

Materials and Methods

Remote sensing data of water bodies was obtained from the Earth Observation portal of EUMETSAT (European Organisation for the Exploitation of Meteorological Satellites) website, which hosts the COPERNICUS Online Data. COPERNICUS is served by set of satellites called Sentinels. Sentinel – 3A was launched on 16th February 2016 and it houses the OLCI (Ocean and Land Colour Instrument). OLCI observation is performed simultaneously in 21 spectral bands, the 1st band has a wavelength of 400 nm, while the 21st (last) band has a wavelength of 1020 nm (Sentinel 3 Marine Copernicus Data Access User Manual, 2017).

The OLCI on board satellite 'Sentinel – 3A', offers water, land and atmospheric geophysical products. These products provide optical observations, in terms of temperature and colour measurements over land and ocean. Chlorophyll concentration data set is a Level 2 geophysical product from OLCI, that indicates algal pigment concentration of water bodies. (Sentinels.copernicus.eu, 2018). WFR denotes the full resolution water and atmospheric geophysical product with a ground pixel of about 300 m at sub satellite point (Sentinel.esa.int, 2018).

After selecting a region of interest (Ireland) and inputting the criteria for advanced search, various WFR images sensed from the period of 1st November 2017 to 31st March 2018 were obtained. The advance search criteria refers to the details about Sensing period, Product type, Timeliness, Instrument name and Product level.

The images were sorted in ascending order of cloud coverage and the images with clear visibility over the region of Ireland were shortlisted. The Costal cover %, Fresh inland water cover %, Saline water cover % and Tidal region cover % details were obtained for the shortlisted images. Then, initial selection was made based on the Saline water cover % and Tidal region cover %, only the images having at least 20 % of Saline water cover and 1 % of Tidal region cover were selected. From the selected images, the best image obtained (in terms of visibility over the region of Ireland and having a good % of Saline water cover and Tidal region cover) in the time period of 5 days was selected (Refer Table 1).

Table 1: Details of selected images

No.	Date	Coastal Cover (%)	Fresh Inland Water Cover (%)	Saline Water Cover (%)	Tidal Region Cover (%)
1	**25/03/18**	**0.175**	**0**	**39**	**1**
2	20/02/18	0.007	1	21	4
3	04/02/18	0.3	0	29	2
4	08/01/18	0.003	0	22	4
5	27/12/17	0.002	0	22	3
6	**15/12/17**	**0.002**	**0**	**41**	**2**
7	08/12/17	0.003	0	26	4
8	29/11/17	0.003	0	32	1
9	23/11/17	0.005	0	22	4

Results and Discussion:

Finally, after the various stages of selection described above, 9 images were obtained (Refer Table 1), and from these 9 images, only 2 images (Details highlighted in bold in Table 1) covered the entire region of Ireland along with its coastal boundaries and thus were selected for the analysis. The first image (Refer Figure 1) was sensed on 15th December 2017 and the second image (Refer Figure 2) was sensed on 25th March 2018.

The time difference between both the images is 100 days. The image sensed on 15th December 2017, has 41 % Saline water cover, 2 % Tidal region cover and, 0.002 % Coastal cover. It has the highest recorded Saline water cover, followed by the image sensed on 25th March 2018, in comparison to the other selected images (Refer Table1). While, the image sensed on 25th March 2018, has 39 % Saline water cover, 1 % Tidal region cover and, 0.175 % Coastal cover.

Further work:

The images sensed on 15th December 2017 and 25th March 2018 will be analysed in MATLAB for obtaining the algal pigment concentration of surface waters in Ireland. The factors that affect and influence the algal pigment concentration will also be studied.

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Figure 1: Image sensed by Sentinel – 3A on 15th December 2017

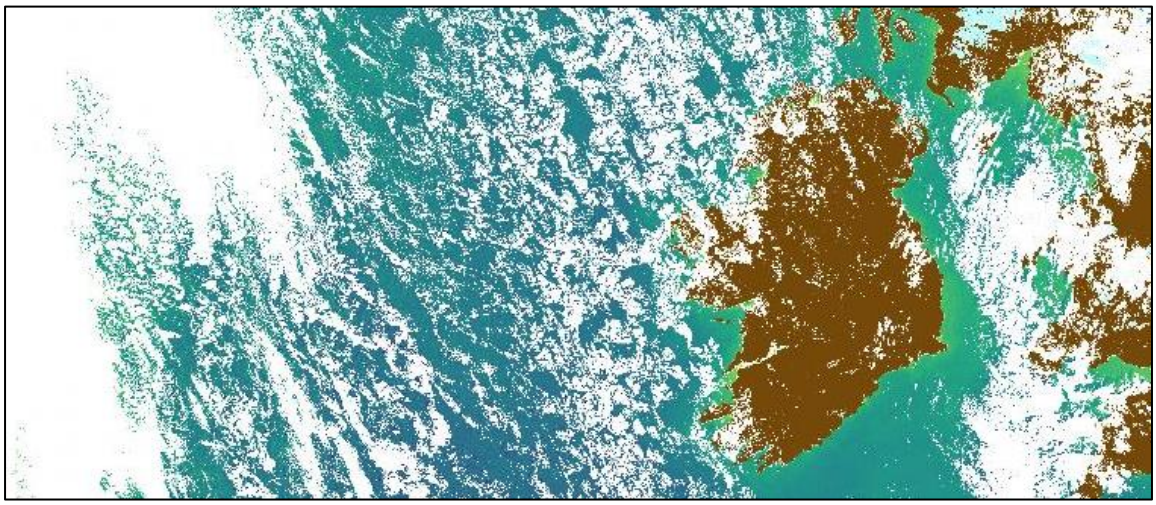
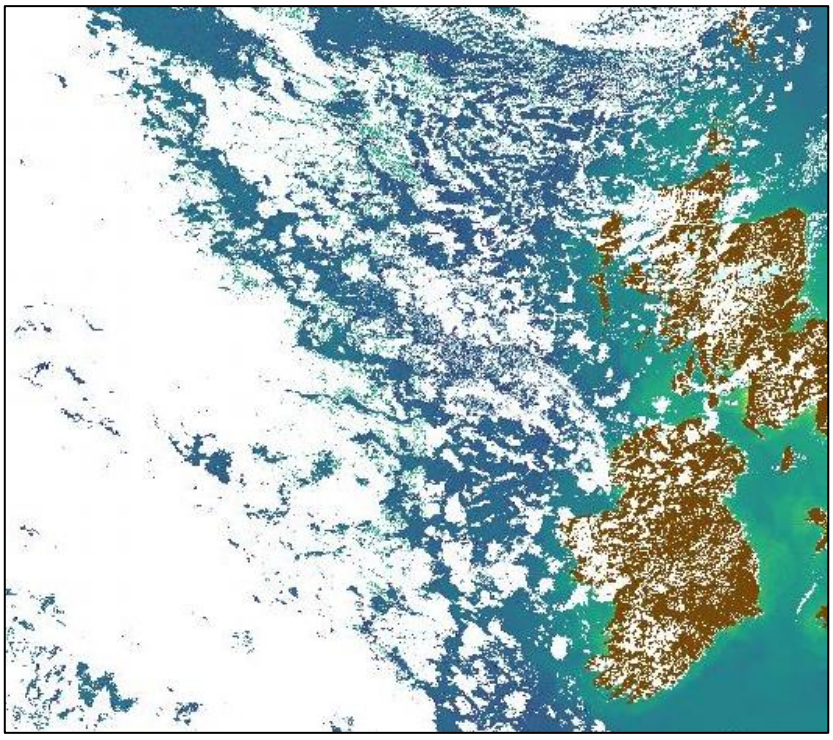


Figure 2: Image sensed by Sentinel – 3A on 25th March 2018



PROVISIONAL STUDY ON THE APPLICATION OF ACETATE- AND PROPIONATE-BIOSENSORS IN FERMENTATION PROCESSES

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Abstract

This preliminary study details the potential applications of previously designed acetate- and propionate-biosensors in commercial fermentation processes. Current monitoring techniques can only detect overloading after it has occurred and are therefore unsuitable for deployment in industry. The sampling of biological leachate and wort samples from anaerobic digestion (AD) and brewing, respectively, in addition to the potential benefits to each process through application of the biosensor, is detailed, with particularly AD of food waste (FW). In addition, future applications in biorefineries is described. Measurement of acetate and propionate allows for greater process control, avoiding overloading and optimising production in commercial fermentation processes.

Introduction

The main objectives of AD are to destroy volatile solids (VS) while producing energy carriers; methane and hydrogen (Sweeney *et al* 2015). To increase efficiency, AD plants are designed to maximise organic loading rate (OLR) and minimise hydraulic retention times (HRT). Waste, such as sewage sludge or FW, can be used as feedstock, resulting in the valorisation of the waste to produce a value-added product (Capson-Tojo *et al* 2016). Volatile fatty acids (VFA), acetate, propionate, butyrate and valerate, are intermediate compounds that appear during the acidogenesis (fermentation) phase of the AD process and are converted into methane by methanogenic bacteria during the final phase (Capson-Tojo *et al* 2016). Current AD monitoring techniques use chemical oxygen demand (COD) or pH, however the degradation rates of propionate and acetate can change before a drop in pH or change in COD reduction efficiency is observed, meaning overloading is only detected after it has occurred (Sweeney *et al* 2015). As a result, there is a requirement for the accurate measurement of individual VFA concentrations, as an indicator of reactor health (Ward *et al* 2008). Total VFA concentrations can be identified with current technologies, however methods for identifying individual VFAs such as acetate and propionate are sparse. For example, Pind *et al* (2003) demonstrated an automated gas chromatography method, however the overall expensive of the system and extensive pre-treatment requirements made it only suitable for large-scale AD deployments (Sweeney *et al* 2015).

A cost-effective solution developed by Sweeney *et al* (2015, 2018), was an acetate-biosensor and a propionate-biosensor, that when operated in tandem, could allow for real time monitoring of acetate and propionate concentrations in an AD reactor. The next step of the development of the biosensors is to test biological leachate samples and explore possible applications for the technology, since it is expected to benefit a variety of fermentation processes so long as acetate and propionate are present and influence the process.

The objective of this study is to explore applications of the biosensors in fermentation processes through the testing of biological leachate and wort samples.

Applications for the Biosensors

Anaerobic Digestion

VFAs, particularly propionic and butyric acids, can inhibit methanogenic bacteria. Propionic acid concentrations of 900 mgL^{-1} (Wang *et al* 2009) and 3000 mgL^{-1} (Boone and Xun, 1987) was shown to be inhibitory and cause system crash, respectively. In addition, acetate:propionate ratios of below 2:1 have been shown to reduce VS destruction and methane production unless hydraulic retention time (HRT) is increased to compensate (Wanger *et al* 2014). Since there exists no mature sensory technology that allows for on-line monitoring of VFA concentrations, avalible to commercial AD operations, many plants are run with a sub-optimal OLR to avoid an overloading crash (Capson-Tojo *et al* 2016). In addition, the use of food waste (FW); or products safe for human consumption that are lost or wasted from food chains (Capson-Tojo *et al* 2016), as a feedstock for AD can be problematic due to its varied nature and rapid biodegradability, which can quickly lead to an accumulation of VFAs and system crash (Capson-Tojo *et al* 2016). FW is an abundant resource, with around one third of total food produced globally becoming waste and this figure is set to increase due to a rise in world population (FAO, 2012). AD represents an improvement on traditional waste disposal techniques, such as landfilling or incineration, that both result in air pollution amongst other negative environmental impacts. AD, particularly with FW as a feedstock, represents an application of the biosensor with potential to make significant improvements in waste management.

Brewing

Another potential application of the biosensor is in the brewing industry. Wort is the growing medium for yeast in the fermentation process, it is rich in nutrients and is made from mashed and heated grain, which converts starch into fermentable sugar (Lodolo *et al* 2008). Wort contains amino acids, synthesised from acids such as acetate and propionate (Macfarlane and Macfarlane, 2003), which are important compounds in the growth of yeast (Lodolo *et al* 2008). Process control depends on the balance of the growth of yeast to produce a consistent product, therefore measurement of acetate and propionate will allow for control of the formation of amino acids, through changes to environmental conditions such as temperature, and ultimately the growth of yeast during the fermentation process (Lodolo *et al* 2008). Like AD, there exists no mature and suitably rapid sensory technology of acetate and propionate, with instead a reliance on a finely tuned process and operator experience to produce a consistent product (Peris and Escuder-Gilabert, 2013).

Biorefineries

Concerns over fossil fuel reserves and the environmental damage resulting from their use, such as greenhouse gas (GHG) emissions, has led to the development of the biorefinery concept, as a long-term replacement for oil refineries (Mohan *et al* 2016). Biorefineries use lignocellulosic biomass, both green and as waste, to produce valuable such as bioplastics and biochemicals (Murali *et al* 2017). Through a series of biological processes, biomass is deconstructed into several high-value products (Lange, 2007), with VFAs acting as platform molecules for fuels, chemicals or other purposes (Capson-Tojo *et al* 2016). Although the biorefinery concept is relatively new, a demonstration plant exists in Austria for the production of lactic and amino acids from grass silage (Ecker *et al* 2012). During this process, the detection of organic acids was completed using chromatography, a slow, lab-based process that does not allow for on-line monitoring. There is a requirement for the development of advanced sensory equipment to match the mature technologies avalible to oil refineries (Mohan *et al* 2016), therefore the biosensor has applications in biorefineries both now and in the future.

Materials and Methods

Biological Samples

Two sources of biological samples, one each from commercial AD and brewing, were identified in this study. Boortmalt, a malt craft beer brewing company with a plant under Minch Malt Limited in county Kildare, will provide the first sample, while Green Generation, a single-phase AD plant with a feedstock of pig slurry and FW, also in county Kildare, will provide the second. Samples are to be transported back to University College Dublin, Ireland, before use and stored at -10°C.

Biosensor and Application

The bioelements developed in the studies by Sweeney et. al, (2015, 2018) were mutated stains of E. Coli, IMD Wldgyep (acetate) and IMD Wldgyepak (propionate), that contained metabolic pathways only for the organic acid being monitored with the exclusion of all others. The whole cell dissolved oxygen uptake of the bacteria, measured with a dissolved oxygen probe, allowed for the acid concentrations to be determined. Screening and successive gene knockouts were performed to obtain only the desired metabolic pathways and were immobilised to improve stability, based on a synthetic leachate (SL) representative of a two-phase AD reactor.

The cell suspensions, 20mg wet cell mL^{-1}, were grown on acetate and propionate as described in Sweeney *et al* (2015). In addition, the method for the oxygen consumption by resting cells will be as described in Sweeney *et al* (2015), with the exception of the use of biological samples, instead of the synthetic leachate in the previous study.

Expected Results and Discussion

The results presented in this section are expected and based on the literature, as no primary data was avalible. The biosensors are expected to successfully monitor acetate and propionate concentrations in biological leachate and wort samples (Sweeney *et al* 2018), continuing the development of the biosensors with a view to deployment in industry. The application of the biosensor in AD is expected to give greater process control, allowing for on-line monitoring of acetate and propionate concentrations in the reactor (Sweeney *et al* 2018). As a result, OLRs could be increased to optimal levels, as overloading would be detected before a system crash and feedstock input or physical operating conditions adjusted to recover (Capson-Tojo *et al* 2016). In addition, favourable acetate:propionate ratios are expected to become easier to maintain, increasing methane production rate and reducing HRT (Wanger *et al* 2014). Furthermore, application in commercial brewing is also expected to give greater process control, allowing for relationships between acetate and propionate concentrations and end product characteristics, such as flavour profile, to be established (Lodolo *et al* 2008). This is expected to allow the operator to make timely adjustments to the physical reactor conditions in order to achieve the desired result. Finally, the sensor is expected to assist in the development of biorefineries, allowing high-value products such as biochemicals to be produced (Mohan *et al* 2016).

Conclusions

Current monitoring technologies are only able to detect overloading after it has occurred and existing technologies for the monitoring of VFA concentrations are not suitable for deployment in industry due to extensive pre-treatment requirements (Sweeney *et al* 2015). As a result, OLRs are often reduced to sub optimal levels to reduce the risk of a system crash (Capson-Tojo *et al* 2016). This is especially significant in the digestion of FW, an abundant and ever-growing resource, due to its rapid biodegradability (Capson-Tojo *et al* 2016). The application of the biosensor in AD will allow for an increase in process control and OLRs and a reduction in HRTs. The biosensor also has potential applications in brewing to increase control of the fermentation step. In addition, biorefineries are required to replace oil refineries as fossil fuels deplete, however a significant barrier is the lack of advanced sensory

technology required to produce products such as biochemicals, which the biosensors can solve in the future (Mohan *et al* 2016).

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FEASIBILITY STUDY OF A COLLECTIVE OFF SITE SOLAR FARM IN ARGENTINA

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Abstract

The current energy crisis in Argentina has driven a new law which provides incentives to generators willing to invest by setting new target growth in renewable energy production over total energy produced. Also the government set consumption targets for users in all the territory to consume 20% of their electricity from renewable sources by 2025. Therefore significant investments in the industry are expected. Quantum America is an international consulting company originated more than 20 years ago in Cordoba, Argentina, and concentrated in utilities regulation. The company is willing to specialize in renewable energy and in this way contribute to that sector growth. Hence, the decision was made to study the possibility of building a solar power plant and offer electricity consumers, especially big users, to supply their target renewable share.

Introduction

Solar power and especially photovoltaic power will potentially play a key role for Argentina to achieve 2025 targets of 20% of renewable energy in the energy matrix (Boudou *et al.* 2015). Due to its favourable solar radiation, the country has a great potential in this area. In fact in 2017, the Argentinian government proceeded to their 3rd public tender as part of the RENOVAR program round 2 that aims to build 1.200MW of renewable energy power stations all over the country (Minem 2018). The 20th of October 2017, national and international actors of the energetic industry answered this public tender by offering more than 9.400MW equivalent propositions (almost 8 times the expected power). The tender was a total success and the solar power was the preferred technology in a power offered base with more than 5.200MW (Minem 2018).

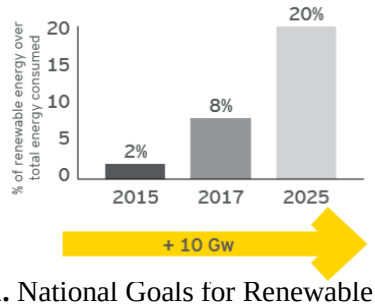

Figure 1. National Goals for Renewable Energy (Pistrelli and Martin 2016)

Additionally to the public tenders, many measures were carried out by the Argentinian government to enhance renewable energy. In a context of energetic crisis, producing electricity from renewable energy sources was declared a national interest. Hence a legal framework was achieved in 2006 (Alberto *et al.* 2006) and intensified since 2015 (Boudou *et al.* 2015) in order to diversify the national energy matrix, expand the installed power capacity and contribute to mitigate the Climate Change. This framework aimed to both developers of renewable energy generation facilities and big users of more than 300 kW of demand. In this favourable context for renewable energy arose the question: What is the best way to build a solar plant and supply electricity to big users at low costs in terms of technic and finance?

The aim of this study is to determine the feasibility of a collective solar power station in multiple regions of Argentina in terms of technology, economy and finance.

Materials and Methods

Electric Production from Photovoltaic

Electric production from PV technology was calculated from solar radiation forecast in multiple locations of Argentina each 30min during the period 2016-2030. Data on solar radiation came from NASA Surface Meteorology and Solar Energy website (NASA 2018). This information was compiled in an Excel Calculation Model in order to determine the electricity production in each location. Also a range of 4 module types, 5 invertor types, 3 structure types and 3 different constructors were considered for the electricity production calculation. That enables the model to be flexible and simulate to 180 different installation setups with different properties for each location. The following tables resume which inputs can be modified in the modelling and what are the technical outputs:

Table 1. PV Modelling input concepts.

Inputs		
Concept	**Unit**	**Value**
Lifetime of the project	años	20,0
Tax lifetime	años	20,0
VAT/IT		Without benefits
Capital cost bti	%	6,00%
Income tax	%	35%
Exchange rate	Euro/USD	0,85
Exchange rate	AR$/USD	18,50
% Funding	%	100%
Term	years	8
Interest rate	%	5,0%
Debit and Credit Tax	%	0,00%
Import tariff	%	0,00%
CO2 generation	Kg CO2/KWh	0,05
Price carbon credit	USD/tn (CO2)	-
Location		Belén-Catamarca
Type of modules		GLC-P6/72
Structure constructor		Clavijo
Type of structure		Un eje
Type of Inverter		Fimer MS 6000 FI
Power factor of design	adim	0,95
Power factor of operation	adim	0,98

Table 2. PV Modelling output concepts.

Outputs		
Concept	**Unit**	**Value**
Net Energy Produced	MWh/año	107.620
Capacity factor	adim	28,6%
Initial Investment	USD	37.024.015
Cost of Land	USD	-
Investment / Total capacity	USD/MW	1.057.829
Area required	ha	129
Power in DC	MW	43
Power in AC	MW	35
Electricity selling price	USD/MWh	48
Tipo de contrato		Cammesa
Capacity factor	MW	0
Annual Profit	USD	1.796.018
% Discount		0%

It can be observed that from specific parameters such as the location, type of modules, inverter, structure and structure constructors, multiples concepts such as the net energy produced, the initial investment, and the area required are calculated.

The next step consists in relate this supply with the demand of big users, and pay a particular attention to the mechanisms of electricity sale (surplus of generation, surplus of demand), regulatory promotional benefits and financial opportunities.

Determination of the demand

The demand of big users interested in the project will be collected and compared to the supply available. Also, a research on public data will be carried out.

Regulatory promotional benefits
The law 27.191 and the decree 531/16 published in 2016 explains the benefits to promote renewable energy. Developers of a renewable energy facility can access tax benefits such as:

- Income tax:
  - Accelerated Depreciation of applicable assets.
  - Tax Loss statute of limitation extended to 10 years (standard is 5 years)
  - Deemed Minimum Income Tax: Temporary exception of the tax
- Value Added Tax:
  - Early refund of VAT Inputs that exceeds VAT outputs
  - Tax credit on locally supplied CAPEX to be applied to the payment of federal taxes
- Other taxes:
  - Exemption of Import Duties

Those concepts will then be added to the modelling to consider a more accurate simulation.

Financial Opportunities
After finding an optimal solar radiation location and technical conditions to build a solar power plant, the installation will be divided in plots of modules available for "renting" for every big user in the geographical area. Each month the electric distribution company will count the energy credits produced per plot to discount it from the customer's bill. This kind of modelling differentiates from other offers since it will work with an assignment of plots. That means customers will not be required any investment.
The study to be achieved will include investigating leads in order to obtain initial investment to build the PV plant. At this stage of the thesis this part is yet to be achieved and I will investigate some leads such as:

- The Argentina Investment and Trade Promotion Agency which an organization that centralizes all efforts to foster and facilitate investment and international trade.
- Project Finance which is a financing scheme in which debt and equity are used to finance an energy project. Argentina already has experience with this type of financing, which is used commonly by oil companies.
- Project for Renewable Energy in Rural Markets (PERMER) which was implemented in 1999 to help the rural low-income areas of Argentina meet their energy needs.

Results and Discussion
Argentina 2025 renewable energy targets are covered in part by the RENOVAR program but one of the purposes of the law 27.191 is also to foster consumers to be part of the transition. The big users shall have to meet the consumption goals individually. To accomplish that purpose, they have different available options:

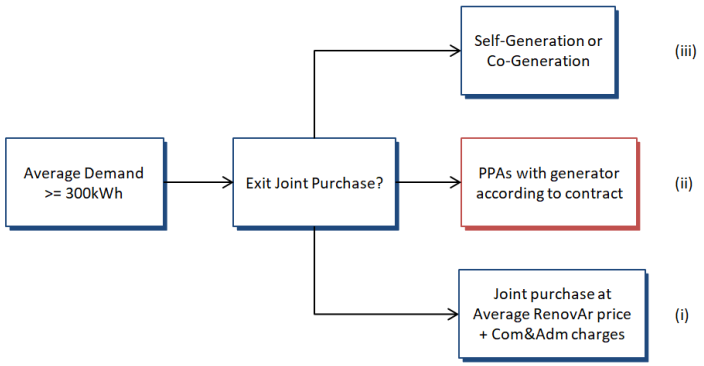

Figure 2. Renewable Electricity Supply options for big users (>= 300kWh) to meet their RE targets.

The choices in order to reach the Consumption Goals are the following: (i) to participate in the joint purchasing mechanism conducted by the Company that Administrates the Wholesale Electric Market Management Company (CAMMESA); (ii) to individually contract electric energy by entering into agreements with private parties (developers, traders and big users); or

(iii) to self-generates or co-generates. This study will focus in the second point power purchase agreement with private parties.

Price

An analysis on prices will be achieved in order to offer the best competitive prices regarding the needs of every customer. Regulation states the price cannot exceed USD 113/MWh (Boudou *et al.* 2015). Also there are two payment alternatives: (a) the "Take or pay" clause, by means of which the off-taker undertakes to pay a fix price during the agreement's validity term, regardless of whether the generated energy is effectively consumed and, on the other hand, the developer undertakes to make available certain amount of energy; and (b) the "take and pay" clause or payment for the effectively supplied energy, in which case, the big user pays a price for each MW of energy effectively consumed. Furthermore, the parties can also agree on a mixed payment structure. Moreover, the excess energy that is not consumed by the off-taker can be sold to CAMMESA up to 10% and, should there still exist a remaining, such remaining can be sold within the Spot Market. This distinction is also important in order to determinate who will be in charge of the imbalances costs.

According to the regulation the price will reflect: (i) tax benefits granted by Law 27,191; (ii) a benefit/ discount in the power reserve fees; (iii) the recognition to the developer of the transport fixed fees; (iv) the release of the payments of fees to CAMMESA for the administration and commercialization services; and (v) the developers' administrative fees as a MEM Agent.

Conclusions

The technical modelling enables to determine which PV installation setup has the best results in terms of costs and technical efficiency for a given location. Also the best results between locations can be compared.

The output of the model shows that returns on investment can vary from 12,4% to 23,9%. However the current calculated scenarios are considering an approximate average price of selling electricity. The next step of the study consists in improving the economic and finance modelling by introducing concepts of PPAs, and promotional benefits in equipment purchasing. Therefore multiple scenarios will be achieved in order to define a transparent and competitive offer for future customers willing to contract electric supply individually.

Acknowledgements

The author acknowledges the assistance of Eng. Damián Halabi at Quantum America, Cordoba, Argentina.

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QUALITATIVE ANALYSIS OF BIOMASS PELLETS USING HYPERSPECTRAL IMAGING

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Abstract

Biomass pellet quality indices will be predicted using a non-destructive biomass pellet characterisation technique known as hyperspectral imaging. Near infrared spectroscopy in conjunction with partial least square regression will be used to predict moisture, ash, carbon and calorific value of the biomass. Range error ratio will be used to find out if the developed model has good to excellent practical utility values. The utilization of such models will aid for the optimal use of feedstocks in the biomass to energy chain.

Introduction

Moisture content present in the biomass directly influences the combustion process, storage management and handling materials. High content of moisture negatively affects the calorific value of biomass leading to inefficiencies(Chadwick *et al.,* 2014). Also, high level of ash content and carbon content impedes the ignition process and affects the calorific value of biomass. Calorific value is nothing, but the chemical energy bound in feedstock and released during combustion process. Development of Rapid, non-destructive Near Image hyperspectral imaging methodology would allow the production of biomass pellets to conform to specific set of standards. Meeting these set of standards would help in reduced variability of the biomass pellets thereby leading to increase in conversion efficiency. As hyperspectral imaging within the NIR region is non- destructive and requires very little sample preparation, it can be used for controlling the quality of renewable carbon materials destined for a wide range of different applications Hyperspectral imaging combines digital imaging and spectroscopy techniques and contains the sample information in two dimensions, spectral and spatial (Mäkelä and Geladi 2017).The image obtained from hyperspectral imaging is made up of contiguous wavebands and each pixel of the image contains an entire spectrum. Thus, Hyperspectral imaging when done in the near infrared region of wavelength 915–1685 nm can be used to predict the quality parameters of the biomass pellets (Gillespie *et al.,* 2016).

The objective of this study is to assess the potential of hyperspectral imaging to predict Ash content (AC), Moisture content (MC), Carbon content (CC) and gross calorific value (GCV) of a multi blend biomass pellet sample.

Materials and Methods

Biomass pellet production
Biomass Pellets were obtained from the Teagasc Crops Research Centre (Oakpark, Co. Carlow, Ireland). The pellets will be produced by inducing the biomass material to a 5 Kw hammer mill with an 8mm screen(Gillespie *et al.,* 2015). The material will then be made to pass through a 6 mm die to take the shape of cylindrical pellets. Before the pelletizing process, the biomass would be blend with different range of biomass materials (Table 1) including Short rotation coppice willow (SRCW), non-woody biomass material, oil seed rape straw and other materials. A small portion of the biomass pellet will be rounded to size of 1 mm for use in the laboratory analysis. The samples will be stored in airtight containers prior to analysis.

Determination of quality parameters
Ash content (AC), carbon content (CC) and Calorific value(CV) will be determined in duplicate according to the international standards (British standards, 2009a, 2009b, 2010).Moisture content will

be determined in triplicate using oven drying method (Plus II Oven, Gallenkamp, Leicestershire, United Kingdom) at 105^{o}C for 24 hours, CC will be determined in duplicate using carbon analyser, AC will be determined in triplicate by combusting the sample in a furnace at 550^{o}C (Carbolite, Hope, England) in accordance with the standard method (Gillespie et al., 2015). Calorific value will be determined in triplicate using a bomb Calorimeter (Parr Instrument, Moline, IL, USA).

Table 1. Percentages of each biomass used in the sample blends.

Biomass	W_{100}	$W_{80}M_{20}$	$W_{60}M_{40}$	R_{100}	S_{100}	$S_{50}M_{50}$	$S_{25}M_{75}$
Wood	100	80	60	-	-	-	-
Miscanthus	-	-	40	-	-	50	75
SRCW	-	-	-	-	100	50	25
Rape Straw	-	-	-	100	-	-	-

Hyperspectral Imaging

Using the push- broom line scanning instrument (DV Optics, Padua, Italy), hyperspectral images of the pellets will be obtained. The instrument consists of moving table, light source, diffuser, mirror, objective lens, a spectrograph (Specim V10E) operating in the NIR range of the spectrum (880–1720 nm); spectroscopic resolution, 7 nm), a CCD camera (580 × 580 pixels), acquisition software (Unscrambler v 9.2; CAMO AS, Oslo, Norway) and a PC (Fagan *et al.*, 2011). In hyperspectral imaging, information is contained in two spatial dimensions and a spectral dimension in the form of a hypercube. Hyperspectral imaging, thus combines both the aspects of spectroscopic and digital imaging techniques to obtain high level of spectral and spatial information of the biomass sample (Gillespie *et al.*, 2015).

Data Processing and Analysis

To carry out the spectral data analysis, wavelength in the range of 950nm to 1671 nm will be taken to eliminate the low signal to noise ratio. The spectra so obtained would be smoothened out with moving average smoothing function with a 5-points segment size. The spectra will then be subjected to first or second derivative steps and multiplicative scatter correction (MSC). Partial Least Squares Regression (PLSR) calibration along with Near infrared imaging will be used to model the moisture, ash, carbon and calorific value in ground samples of biomass pellets. Unscrambler Acquisition software (v 9.2; CAMO AS, Oslo, Norway) will be used to develop prediction models for the determination of AC, CC, CV and MC (Fagan *et al.*, 2011). Full cross validation will be employed, and the root mean square error of cross validation (RMSECV) would be obtained. Range to error ratio (RER) will then be calculated by dividing the range of the independent variable by the prediction error for that variable and would be used as a standard reference for room mean square error values (RMSE). Calibrated models having RER values of less than 3 would be considered very poor and should not be considered for any application, models with an RER of between 3 and 10 indicates limited to good practical utility and could be used in a screening application and values above 10 shows that the model has an excellent utility value and could be used in any application (Fagan *et al.*, 2011).

Results and discussions

Prediction of Moisture content (MC)

Previous studies have shown that eliminating the visible spectra from the full spectral range resulted in the strongest model (RMSECV = 0.90%, $R2$ = 0.99, RER = 39.3, RPD = 13.5) as seen in Figure 1a. The $R2$, RER and RPD all indicate an excellent prediction model which could be used in any application. The first three loadings in the mode, Figure 1b account for 92%, 6%, and 1% of the variance in the spectral and 92%, 6%, and 1% variance in the reference data respectively (Fagan *et al.*, 2011). The loadings shown in Figure 1b are derived from 1st derivative spectra.

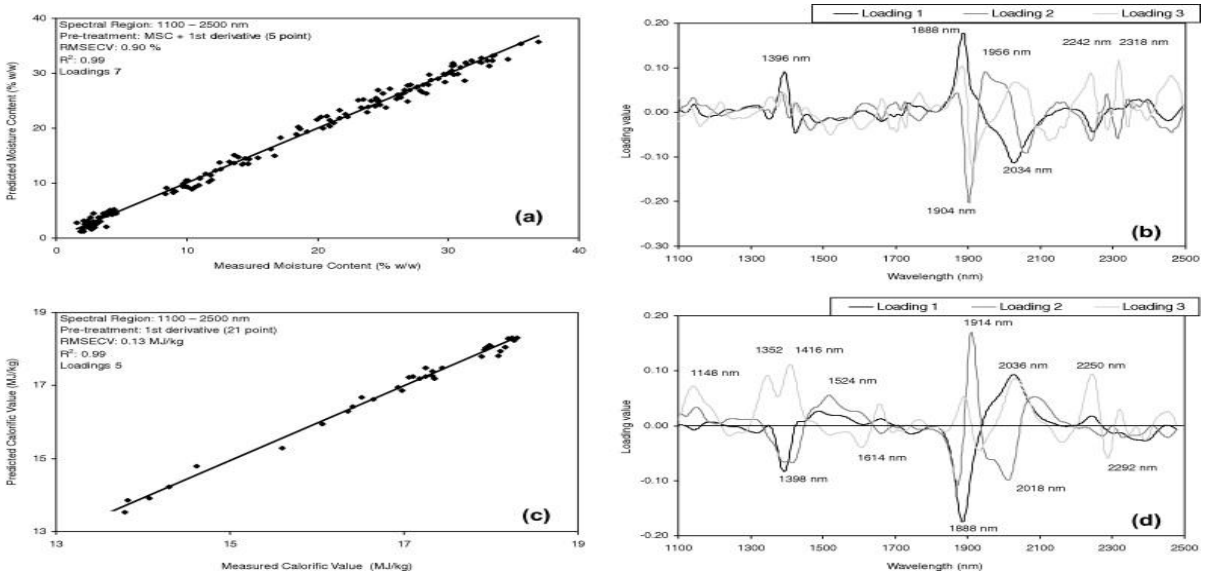

Figure 1 Linear regression plots of predicted versus actual (Fagan *et al.,* 2011) (a) moisture content and (c) calorific value of SRCW and *Miscanthus* samples and PLS loadings plot for loadings 1 (——), 2 (——) and 3 (——) for PLS models of (b) moisture content and (d) calorific value prediction (Fagan *et al.*, 2011).

Prediction of Calorific value (CV)

In accordance with the previous studies, prediction of calorific value was done using NIR spectroscopy and PLS regression. The best model was developed using the full NIR range although using the full visible-NIR spectra also provided an excellent model and used two less loadings (Fagan et al., 2011). RMSECV value (0.13MJ/Kg), *R*2 (0.99), RER (39.9) and RPD (70.8). Figure 1c indicated that as with moisture, the developed model had an excellent fit with the data and could be used in any application (0.13 MJ/kg), *R*2 (0.99), RER (39.9) and RPD (70.8) (Fagan *et al.,* 2011) . This model was developed using 1st derivative spectra and unlike the moisture prediction model did not employ scatter correction. Figure 1d shows the first three loadings employed in the model (Fagan *et al.*, 2011).

Prediction of Ash content (AC)

Ash content was determined on wet and dry basis. The best predicted model was obtained using the NIR region 750 to 1100 nm) which had been pre-treated using MSC and a 1st derivative step (Fagan *et al.,* 2011). Ash on wet basis was the weakest prediction model developed for any parameter (RMSECV = 0.42%, *R*2 = 0.58, RER = 7.7, RPD = 3.6) (Fagan *et al.,* 2011) as shown in Figure 2a. The first three loading in the model Figure 2b account for 50%, 46%, and 3% of the variance in the spectral data and 27%, 12%, and 22% variance in the reference data respectively. Figure 2b gives the ash content prediction in the spectral regions -970 to 974 nm and 1100 nm.

Prediction of carbon content

Like Ash prediction, carbon content was also predicted on dry and wet basis. Carbon content on dry basis is not taken into account as it shows similar value to the ash model on dry basis (Fagan et al., 2011). Carbon content on a wet basis was best predicted using 2nd derivative spectra in the range 1100 to 2500 nm. The prediction statistics for the model (RMSECV = 0.57%, *R*2 = 0.88, RER = 10.4, RPD = 4.6) Figure 2c suggests that the accuracy of the model is fair, and it could be used in a screening application. The first three loading in the model Figure 2d account for 72%, 8%, and 17% of the variance in the spectral and 75%, 10%, and 1% variance in the reference data respectively. Numerous wavelengths were found to be important in the prediction of carbon content as shown in Figure 2d (Fagan *et al.,* 2011).

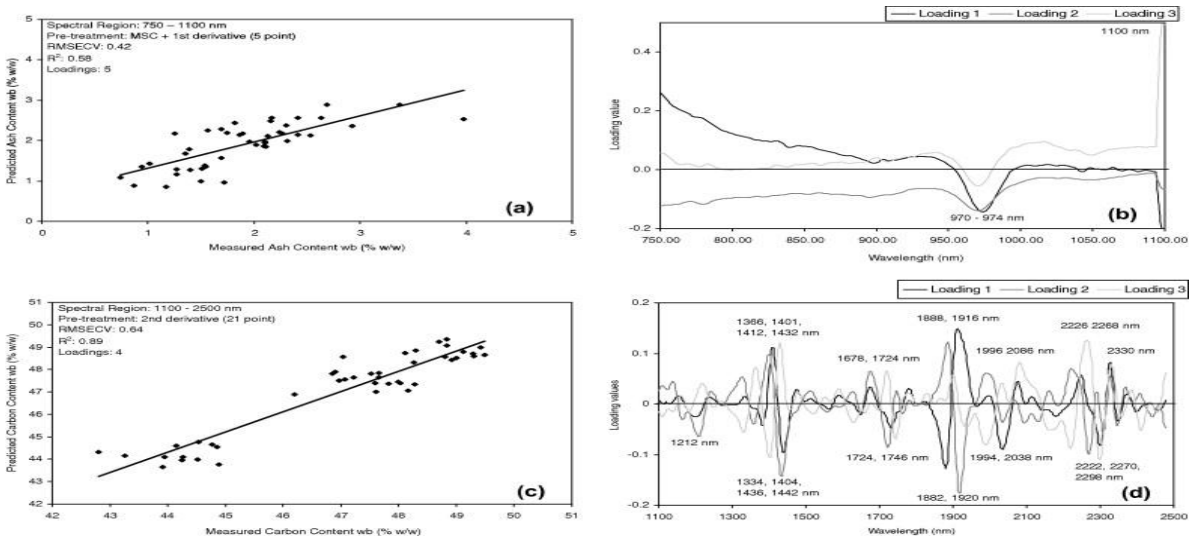

Figure 2. Linear regression plots of predicted versus actual (Fagan *et al.*, 2011) (a) ash content on a wet basis and (c) carbon content on a wet basis of SRCW and *Miscanthus* samples and PLS loadings plot for loadings 1 (━━━), 2 (——) and 3 (——) for PLS models of (b) ash content on a wet basis and (d) carbon content on a wet basis prediction (Fagan *et al.*, 2011)

Conclusions

By using the calibration and validation models, prediction of the quality parameters of biomass pellets like moisture, carbon content, ash contents and gross calorific value is possible. The results show that NIR hyperspectral image is a non-destructive technology to assess the quality constraints of biomass pellets. This would allow for on-line systems to be developed for a biomass to energy system.

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PRELIMINARY ENERGY CONSUMPTION REVIEW AND CARBON FOOTPRINT ANALYIS OF THE MARBLE ARCH CAVES

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Abstract

The aim of this paper is to improve the energy efficiency of the Marble Arch Caves and its visitor centre. As the building has not yet been assessed for its efficiency and hence possible savings, a case study of a similar building was used to predict decreases in electricity consumption. Once possible savings are applied to current energy consumption trends, HOMER software was used to suggest which renewable energy systems are the most suitable in terms of both economic feasibility and increasing the renewable fraction, with the carbon emissions of each system considered. When more data is available, this paper will also consider improves to the current heating system and heat retention, as well as considering the carbon footprint of the vehicles used by the caves and possible improvements.

Introduction

The Marble Arch Caves Global Geopark, County Fermanagh, was established in 1985 by the Fermanagh District Council (now the Fermanagh and Omagh District Council). In 2001, the cave and surrounding Cuilcagh Mountain Park were awarded with European Geopark status in 2001, which was upgraded to Global Geopark status in 2004. Since that date the Geopark was constantly expanding, eventually establishing sites in County Cavan, making it the Global geopark to span an international border. This continued expansion resulted in the Geopark being awarded UNESCO status in 2015, with over 40 sites throughout the geopark. The main site is the Marble Arch Caves themselves, consisting of the caves themselves and an above ground visitors centre (Marble Arch 2018).

Due to the size of the caves and the visitor centre and the length of the tour season (March-November). This means that a significant amount of electricity is consumed, and therefore money spent, in keeping the caves operating, with the 2017 season resulting in a usage of 100,867 kWh and an expenditure of €14,748. **The objective of this study is to make the Marble Arch Caves more energy efficient and subsequently increase the renewable fraction of their energy consumption to lower costs in the long run.**

Materials and Methods

Increasing Energy Efficiency

The current energy usage statistics for the MAC visitors centre can be seen in Figure 1. Once a full assessment of the visitors' centre and the caves has been completed, measures will be suggested to increase energy efficiency in the building and reduce the overall energy usage. There will be a range of efficiency measures suggested, such lighting and behavioural programmes. Using a similar method and including daylight detection lighting systems, luminaires and task lighting, AGET manufacturing reduced its electricity spent on lighting by 75%, which is typically only achievable in business that have large energy expenditures on lighting, similar to the Marble Arch Caves (Hestnes & Kofoed 2002). If the same energy percentage was applied to the Marble Arch Caves, and it is assumed that 40% of the caves energy expenditure was on lighting as suggested by Electric Ireland (2018), this could result in a significant decrease in energy consumption. Other methods of increasing efficiency will also be considered.

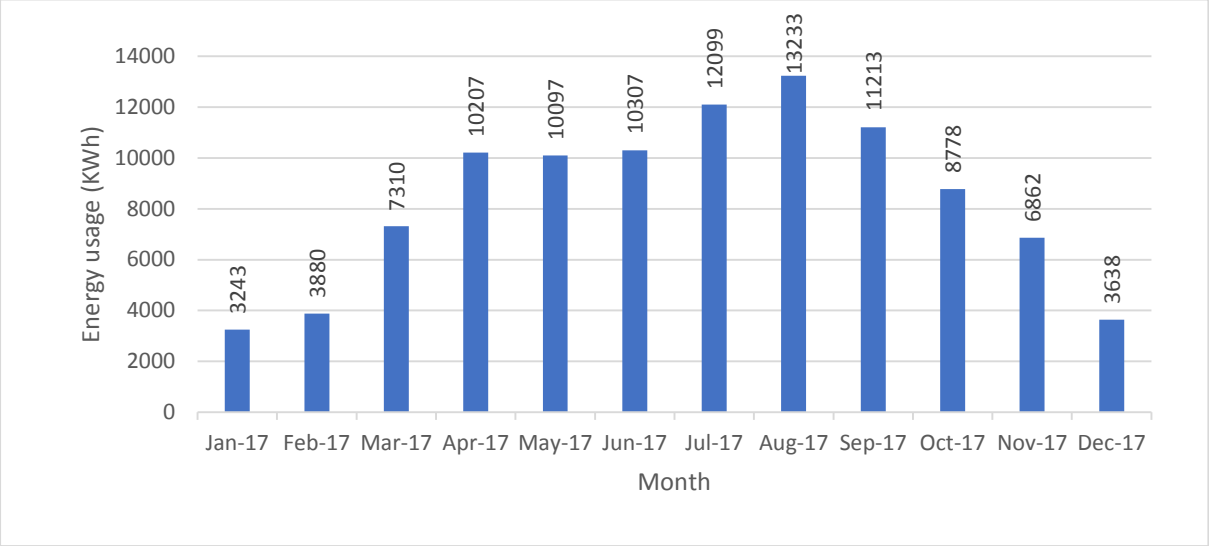

Figure 1: Energy consumption statistics per month for the Marble Arch Caves

Increasing the renewable fraction of energy

At the early stage of this report, PV and Wind will be the only green technologies to be considered in increasing the renewable fraction of the energy consumption, although this could possibly include hydro energy as the river in the cave floods frequently and has a high discharge that could potentially be harnessed. A preliminary model will be constructed using HOMER software, and the data inputs for the wind and solar resource can be seen in Table 1. Currently, SSE Airtricity supply the electric for the cave and claim to have an energy mix that is 36% sourced from renewables and 64% from natural gas.

Table 1: Data inputs for wind and solar resources in HOMER

	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OVT	NOV	DEC	AVG.
Wind Speed (m/s)	6.03	7.70	6.47	5.66	5.21	6.47	4.25	3.01	3.45	4.13	3.01	6.16	5.11
Solar Irradiance (kWh/m^2/d)	0.50	1.00	2.03	3.53	4.19	4.30	3.71	2.87	2.36	1.32	0.63	0.39	2.24

Reviewing the heating system

The visitors centre is currently heated by a wood chip boiler installed in 2015. While no data has been provided on this system yet, it is at the higher end of efficiency in terms of heating systems. However, (Ming To et al. 2014) suggest that while wood chip boilers are efficient, air source heat pumps are much more efficient (300% to 85% if measuring Energy Out/Energy In) and while they have higher initial costs, they have lower operating costs. The feasibility of installing such as system will be assessed at a later stage.

Reducing Carbon Footprint

Currently, the only available information in which to make an assumption about the overall carbon footprint of the caves is electricity data. Once data for heating systems and company vehicles (in terms of fuel efficiency and annual distances travelled) is collected then a better understanding of total CO_2 equivalent emissions can be gained.

Results and Discussion

If improvements to energy efficiency as suggested previously are correct, a preliminary prediction of possible energy consumption trends in the future of the MAC can be seen in Figure 2. The new total is down from 100867 kWh/year to 72,624 kWh/year.

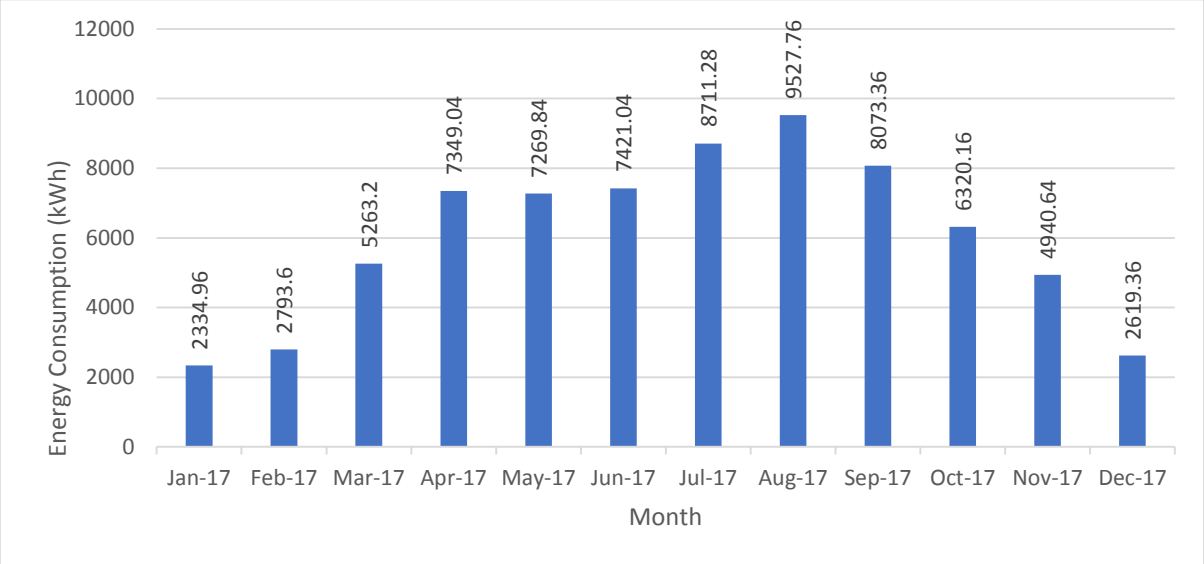

Figure 2: Predicted reductions in the energy consumption of the caves

For the current time, only PV panels and Wind turbines in a grid tie system were considered in improving the renewable fraction of the caves energy consumption. HOMER software was used to construct preliminary optimal models for the caves in terms of improving renewable fraction and economic feasibility. Wind resource data was collected by selecting the nearest anemometer and using wind shear data as provided by (Ray et al. 2006) to extrapolate for possible wind speeds at the site of the caves, which is 120m higher than the sire of the anemometer. Solar data was obtained from PVSol.

The economic breakdown and renewable fraction of each system as suggested by HOMER can be seen in Figure 2, which assumes the predicted energy consumption, and not the current consumption. Note that figures in US$ actually represent GBP (£).

PV (kW)	G10	L16P	Conv. (kW)	Grid (kW)	Initial Capital	Operating Cost ($/yr)	Total NPC	COE ($/kWh)	Ren. Frac.
30			12	1000...	$ 17,675	8,186	$ 222,327	0.123	0.29
30		2	12	1000...	$ 18,275	8,252	$ 224,577	0.124	0.29
				1000...	$ 0	9,652	$ 241,295	0.134	0.00
		2	4	1000...	$ 1,492	9,822	$ 247,031	0.137	0.00
30	1		12	1000...	$ 52,675	8,579	$ 267,140	0.148	0.39
30	1	2	12	1000...	$ 53,275	8,645	$ 269,390	0.149	0.39
	1		6	1000...	$ 36,337	10,138	$ 289,781	0.160	0.12
	1	2	6	1000...	$ 36,937	10,204	$ 292,031	0.162	0.12

Figure 3: HOMER analysis for optimal systems including PV and Wind systems

HOMER suggests that economically, the most feasible system is a 30kWp PV system with no batteries. However, this is disregarded as there in a need for energy storage for surplus energy generated. Considering it only costs £2,350 extra over 25 years for 2 batteries, a system including the grid, a 30 kWp PV system, 2 batteries and a 12kW converter is assumed to be optimal economically,

with a net present cost of £224,577 and £0.124/kWh, compared to sticking with a grid only system, which has a net present cost of £241,295.

In terms of the most optimal system for increasing the renewable fraction of energy, a system of the grid, a 30kWp PV system, a 10kWp wind turbine and a 12kW converter is the most optimal, with a renewable fraction of 0.39 (as HOMER doesn't consider the grid mix, including the fact that SSE Airtricity already claim that 36% of their mix is renewably sourced, the total renewable fraction is approximately 0.61). The carbon footprints of the above systems are expressed in Figure 4. This doesn't consider heating systems or vehicles in use by the MAC and this will be considered at a later stage.

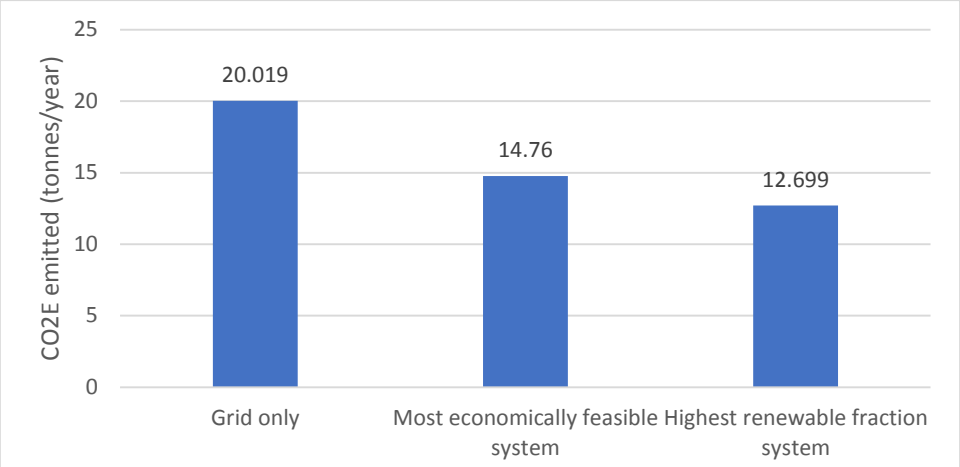

Figure 4*:* The carbon footprints of the previously described systems

Conclusions

This paper concludes that the Marble Arch Caves can likely reduce overall electricity consumption, increase the renewable fraction of their energy consumer while remaining economically viable and reduce their carbon footprint. Further development of this report will also include a look at the feasibility of using hydro turbines to harness the river energy, an upgrade to the pre-existing heating system and reducing the carbon emitted from vehicles used.

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THE ROLE OF SOLAR PV IN IRELAND'S FUTURE ENERGY SYSTEM

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Abstract

The incorporation of greater amounts of solar photovoltaic (PV) into Ireland's energy system is becoming increasingly plausible. The current national energy system is unsustainable, due to over-reliance on fossil fuels. This research collects and analyses data from various factors that affect the efficacy of solar PV technology in Ireland. The findings are used to discuss any potential hindrances and possible resolutions to the integration of solar PV in Ireland's future energy system. It is concluded that solar PV offers a partial solution to Ireland's energy and sustainability issues as it can provide cost-effective, low-carbon energy to the system.

Introduction

Ireland's current energy system is based primarily on imported fossil fuels. They form the foundation of energy use in all sectors from transport to agriculture, and fossil fuel demand is growing by an average of 5% annually (SEAI 2017). In 2016, final energy consumption in Ireland reached a total of 14.41 Mtoe, of which fossil fuels accounted for 92%. The transport sector consumes the largest portion of energy (35%), followed by residential and industrial (24% each), services (14%) and lastly agriculture/fisheries (2%) (SEAI 2017). As of December 2015, Ireland and 195 other parties entered into the Paris Agreement in a global agreement to mitigate climate change and keep global warming levels below 2˚C. Ireland's 2020 EU targets state that 16% of final energy consumption from all sectors must come from renewable sources, and that GHG emissions must be reduced by 20% from 2005 levels (by approx. 68 Mt CO_2). If Ireland fails to meet these targets, which seems likely, they will face a €75 million fine annually, until the targets are met (SEAI 2017). If Ireland are to meet their future targets, the country's energy system must be completely changed from a fossil fuel-based society to one that is based around Renewable Energy Systems (RES). In 2016, renewable energy supply slightly increased by 0.3% from the previous year, accounting for 8% of the total national energy supply (SEAI 2017). Ireland has a long way to go before it can achieve a society based on renewable energies, and the present rate that it is changing is far too slow.

Currently, solar plays a minute role in the supply of the country's renewable energy, a mere $6MW_p$ installed on commercial and residential rooftops (SEAI 2017). There are currently no solar farms in operation in Ireland. However, the market for solar is rapidly growing, due to the emergence of new technologies (Green *et al.* 2014), increasing solar cell efficiencies (Baquedano *et al*. 2017) and the swift decline in the cost of PV panels (Bolinger *et al*. 2015). Solar PV is positioned to become one of the most important energy technologies in meeting global sustainable energy and climate commitments. Sweden for example, as of 2016, installed solar PV capacity surpassing 205 MW (SEA 2017). Sweden is located at an even higher latitude than Ireland, thus it receives less direct sunlight. Any Irish person knows that the Sun doesn't shine all day long or all year round, and this leads to the pessimistic view that the Irish climate isn't suited to solar PV. With continuously improving storage technologies, the problem caused by the fluctuating nature of the Sun can be largely diminished (Li *et al.* 2017). If Ireland is going to play its part in the mitigation of dangerous levels of global warming, the country needs to take a leaf from Sweden's book and commit to solar as a key source of renewable energy. **The objective of this study is to investigate the limitations and solutions to the integration of solar PV into Ireland's national energy system.**

Materials and Methods

Data from many different factors, which influence the role of solar PV in the country, is collected and analysed. This data pertains to Ireland's current energy system, solar irradiation levels, PV technology, the price of PV modules, and the availability of land in Ireland.

Ireland's Current Energy System

The 2016 (most recently published) national energy data is obtained from the SEAI's (Sustainable Energy Authority Ireland) energy balance report (SEAI 2017). The flow of energy in Ireland in 2016 is portrayed in Fig. 1, showing both energy supply (renewable and fossil fuels) and demand (transport, residential etc. sectors). Oil (48%) and natural gas (29.5%) supply most of the country's energy. These fossil fuels are well-established and facilitated, and this has led to renewables, such as solar PV, being somewhat neglected in Ireland (ISEA 2017). In general, electricity infrastructure in Ireland is well maintained and safe, conforming to international standards. However, more flexible power generation and electricity storage will be needed in the future to match the intermittency of renewable electricity. Presently, Ireland's infrastructural system is not advanced enough to incorporate decentralised solar PV on a national scale (Engineers Ireland 2016).

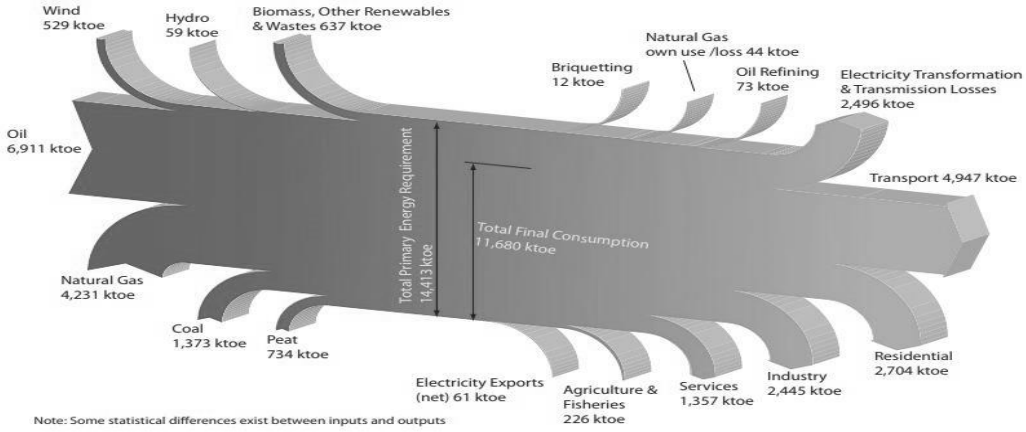

Figure 1: Energy flow in Ireland in 2016 (SEAI 2017).

Solar Irradiation in Ireland

Solar irradiation data is sourced from Met Eireann, the Irish National Meteorological Service. Ireland typically receives between 1100 and 1600 hours of sunshine annually. The southeast of the country receives the most hours of sunlight (Met Eireann 2018). Fig. 2 shows the average annual sunshine in hours for the country. The darker the area, the more sunshine it receives on average. Using the Global Solar Atlas, it was determined that solar PV in Ireland has comparable capacity output to countries such as the UK and the Netherlands (850-950 kWh/kW_p per year) (WBG 2018).

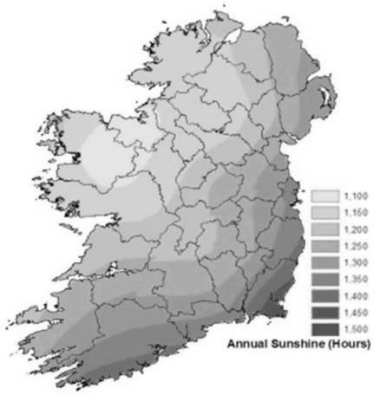

Figure 2: Annual sunshine hours in Ireland (Met Eireann 2018).

Solar PV Technology
According to the International Energy Agency (IEA), in 2016 solar PV grew faster than any other energy source in the world, its capacity increasing by 50%, (78 MW) (IEA 2017). This huge leap in installed capacity is mostly due to China's dramatic increase in PV production (IEA 2017). The installed global PV capacity is now almost 400GW, and this number is on the rise. Fig. 3 shows the amount of PV capacity that has been installed each year since 2007 and the amount projected to be installed up to 2022.

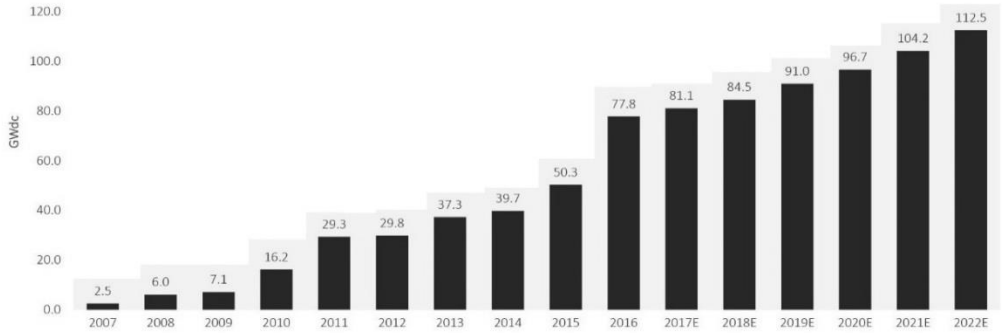

Figure 3: Global installed PV capacity by year (IEA 2017).

The efficiency of a variety of research-cell PV technologies was neatly summarised by the National Renewable Energy Laboratory (NREL). Most crystalline Si cells have efficiencies between 21% and 27%, while some multi-junction cells have exceeded 40%. Emerging technologies, such as Perovskite cells, have rapidly increased in efficiency over the past few years (NREL 2016). Many of these technologies have yet to enter the market and there is plenty of opportunity for these improved efficiency cells to do so in the near future.

Price of PV modules
With the huge increase in PV production, comes a rapid decline in the price of silicon modules. The price of solar PV has decreased by around 80% from 2008 prices, according to the International Renewable Energy Agency (IRENA). In India, the price of a PV system now stands at a record low of approximately €0.5/W, while the average price in Europe is around €0.75/W (IRENA 2018). The exact cost of solar PV in Ireland has not been determined due to the relatively small levels of installed capacity.

Availability of Land
In the past two years, over 250 planning permission applications for solar farms have been made in Ireland. A combined total of more than 25,000 acres of land has already been put forward for the development of solar farms. Planning permission has been granted for many farms and their operation will commence within the next year or so (Harmony Solar 2018).

Results and Discussion

Solar Energy Source
There are many potential obstacles to the integration of solar PV in Ireland. The most obvious is the fluctuating nature of the Sun. Solar energy varies depending on the time of day, the season and the weather, thus it is not a constant source of energy. However, this problem can be solved with the use of storage. Storage technologies are constantly being updated and improved, and there are many options available, including batteries, pumped hydroelectric and compressed air storage (Child *et al.* 2017). The cost of lithium-ion batteries is rapidly declining due to their large-scale production in the motor industry, making them one of the more beneficial options to choose from (Li *et al.* 2017). The improved efficiency and the increased available capacity of the PV technology itself also help to overcome this obstacle. The combination of these advancements allows for greater energy generation than before. Countries with similar levels of sunshine to Ireland, such as the UK and Denmark, already

have mature solar PV industries. This suggests that it is very possible for Ireland to develop a successful PV industry.

Ireland's Economy

Another significant barrier to solar PV is that there are no financial subsidies for solar PV in Ireland, and no national REFIT scheme, making solar less competitive in Ireland than other renewable energy sources. There are no feed-in tariffs for micro-generated solar PV at the moment, but a microgeneration bill is currently being assessed in parliament. Organisations who are promoting the development of sustainable energy policies, such as the Irish Solar Energy Association (ISEA), are gaining recognition. Financial aid from the government is key for the growth of solar PV in Ireland. The constantly dropping price of silicon PV systems globally will make solar PV much more attainable in Ireland and will help ensure its economic viability.

Conclusions

To date, Ireland has only scratched at the surface of solar PV. Solar PV is the fastest growing renewable technology in the world and the global installed capacity is now almost 400 GW. The price of silicon-PV panels is also declining rapidly, making them more available now than ever before, and this is expected to continue. Acres of agricultural land are available for the development of large-scale solar farms. Storage technologies are becoming more prevalent in the industry, and financial aids are likely to be available in the near future. All of these trends point to one prospect; solar PV is poised to become one of the key energy sources in Ireland's future energy system.

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REACHING THE TARGET FOR ELECTRIC VEHICLES IN EUROPE: DEPLETION OF METALS USED IN EV BATTERIES

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Abstract

An increase in the popularity of electric vehicles (EV) leads to an increase in demand for EV batteries. The leading technology in electric vehicle batteries is currently lithium-ion, used in the vast majority of EVs manufactured today. This study quantifies the metals needed for the production of lithium-ion batteries, and the resource availability of those metals to analyze the extent of the metal depletion, if Europe was to reach the target for electric vehicles by 2050. The study also explores the possible recycling options for lithium-ion batteries. The expected results should prove that the depletion of some of the earth metals maybe cause problems for the automotive industry. It should also identify more efficient and feasible recycling methods, which will prevent the need for heavy resource extraction and minimize battery waste.

Introduction

Countries all around the world are working towards a greener future and a decrease in greenhouse gas emissions (United Nations 2016). This is a necessary change to help minimize the negative effects of climate change. Even with such advanced technological improvements, like the introduction of electric and battery powered hybrid vehicles, or the expansion of public transport systems, the transport sector in Europe accounts for a quarter of the continent's greenhouse gas emissions. It is also a huge contributor to the low air quality standards and noise pollution among European cities (European Environment Agency 2016). One of the steps taken to help this crisis is the shift from internal combustion engines (ICEs) to battery electric (BEV) and plug-in hybrid electric vehicles (PHEV). A number of measures are being implemented on a national and European scale to encourage people to buy electric vehicles like; low cost or free charging stations or grants for newly bought electric cars (European Environment Agency 2016). The EU released the Transport White Paper in 2011, in which they outlined a plan to reduce the GHG emissions in the transport sector by 60% by 2050, relative to the emissions from year 1990. The paper shows how this can be achieved to hopefully decrease the continent's reliance on oil. To reach this target, the EU is hoping to halve the amount of conventionally fueled cars driven in cities by 2030 and completely eliminate them from urban areas by 2050 (European Union 2011).

The shift to battery powered vehicles carries a different environmental burden. The lithium-ion battery packs which are currently used in most of the electric vehicles manufactured today, require a number of rare earth metals for their production. These metals include; lithium, aluminium, manganese, nickel, and many more, and they are essential not only for the automotive industry but for many other industries around the world (Witkamp *et al* 2017). It is essential that they are extracted and used in a sustainable way to prevent shortages worldwide. To prevent over extraction, old batteries could be recycled, and some of the essential metals could be reused for the production of new batteries. At the moment, a lot of the recycling techniques for lithium-ion batteries are not energy or cost efficient, making them unfeasible. A new more efficient method could greatly reduce the need for heavy metal extraction but also, minimize the waste produced by old and unusable lithium-ion batteries (Xu *et al* 2008). **The objective of this study is to assess if the shift to battery electric vehicles, is a sustainable option for the reduction of greenhouse gas emissions within the transport sector in Europe, from the perspective of the depletion of metals used in EV batteries. It will also cover the feasibility of potential recycling options for those lithium-ion batteries.**

This will support one of the EU Circular Economy Strategies proposed at the start of 2018, which involves a Report on Critical Raw Materials and the circular economy (Ec.europa.eu 2018).

Materials and Methods

Target for Electric Vehicles in the European Union and Current Status

In 2016, only 1.2% of all newly bought passenger vehicles in the European Union were electric. They accounted for only 0.15% of all the cars in Europe that year (European Environment Agency 2018). To reach the targets set by the EU those percentages have to increase rapidly. Over 15 million passenger vehicles were registered in the EU in 2017 (European Automobile Manufacturers Association 2018). According to forecasts, the sale of BEVs will rise to around 30% of total car sales in the EU by 2050. The forecasts also predict, that from now until 2020, the sales of electric vehicles will be steady, at around 1.2%, and then will rise linearly as shown in Figure 1 (Witkamp *et al* 2017).

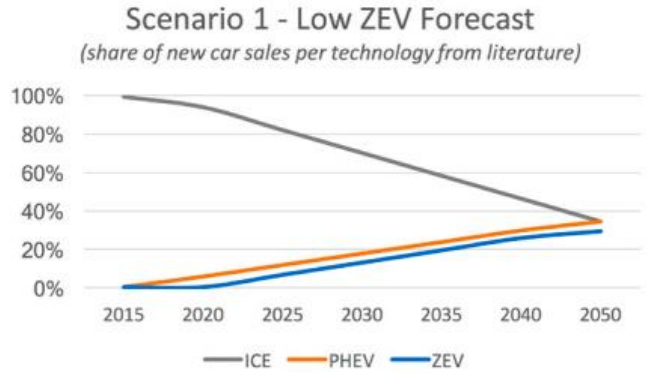

Figure 1. Forecast for Electric Vehicle Sales in the EU (low rise of sales) (Witkamp *et al* 2017)

If it is assumed that the same number of passenger vehicles will be bought every year between now and 2050, there will be a requirement for nearly 74 million electric vehicles in the European Union alone. To complete this project, ten of the best-selling electric cars in the EU will be analyzed and their battery types identified, and they are listed in Figure 2.

Table 1. Top 10 Best Selling EVs in the EU in 2018 (Eafo.eu 2018)

Make	Model	Battery Type
Renualt	Zoe	Lithium Ion
Tesla	Model S	Lithium Ion
BMW	i3	Lithium Ion
VW	e-Golf	Lithium Ion
Tesla	Model X	Lithium Ion
Hyundai	IONIQ Electric	Lithium Ion
Kia	Soul EV	Lithium Ion
Smart	Fortwo ED	Lithium Ion
VW	e-Up!	Lithium Ion

Electric Vehicle Batteries

Large battery packs are required to power the electric vehicles listed above, and at the moment, lithium-ion is the leading battery technology used among the majority of EV manufacturers. For the purpose of this study, 5 different types of Li-Ion batteries will be analyzed; Lithium-Iron Phosphate, Lithium-Titanate, Lithium-Manganese Oxide, Lithium-Nickle-Cobalt-Aluminium Oxide and Lithium-Nickle-Cobalt-Manganese Oxide. The majority of the materials used in these batteries are similar, the main component that differs is the active substance in the cathode; the negative electrode within the battery.

Quantitative Study of Metals in EV batteries
In order to see if the shift to electric vehicles is sustainable, a quantitative study of metals used in the batteries listed above will be completed. These metals include; lithium, aluminium, zinc, copper, cobalt, nickel, iron, manganese, etc. (Peters and Weil 2016). To quantify these metals, a thorough analysis of the currently available data on the five lithium-ion batteries will be analyzed and grouped in Microsoft Office Excel. The weight fractions of each metal will then be multiplied by the assumed amount of batteries required by 2050 in the EU. Once this data is obtained, a resource availability study will be performed.

Resource Availability
The next stage of the project involves completing a resource availability study of the metals used for the production of the batteries. This will be done by analyzing currently available information related to the specific metals in published journals, books and articles. From preliminary studies it is obvious that the availability of resources like lithium is not completely certain and due to the locations where the ore is found and its uneven distribution, geopolitical tensions might result in its shortage. Nevertheless, the known supply of lithium in the world should not be a cause of problem for the automotive industry (Oliveira *et al* 2015). The full study will show, if any of the other metals used are in short supply and will cause issues in future manufacturing of lithium-ion batteries.

Recycling Options for EV batteries
There are a number of ways in which lithium-ion batteries can be recycled. It is argued that some of the processes might not be eco-friendly, they require a large amount of energy and are not very cost effective. The recycling methods divide into two types of processes; physical and chemical. The full process of recycling a battery pack involves a mixture of different types of processes, as shown in Figure 3 (Xu *et al* 2008)

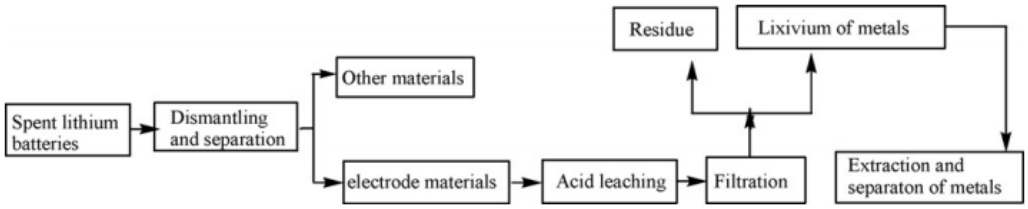

Figure 2. Process diagram of a typical recycling process for a lithium-ion battery (Xu *et al* 2008)

Results and Discussion

The work for this project is on-going, and no final results are available yet. Thus, this section includes only provisional results and assumptions. The expected result of this study is that;

- There might be a shortage of some of the rare earth metals once the amount of manufactured electric vehicles increases,
- Geopolitical tensions around the world might cause a shortage of specific metals, due to the fact that resources are not evenly spread around the world,
- New technologies will have to be developed to replace lithium-ion batteries, even if there is enough resources to continue the production in Europe until 2050,
- New, efficient recycling methods are available to recover some of the metals from used lithium ion batteries.

Conclusion

Regardless of the final results of this study, new technology should be developed to minimize the use of natural resources in the energy sector. The current technology does not fulfill the demands of the growing population, and the technologies that are being developed and becoming widely used still highly exploit the world's resources. Metals are extremely valuable substances in the world, across all different industries, so it is crucial that they are used and extracted in a sustainable and smart way. The road transport sector is growing every day and the development of new passenger vehicle technologies will be important to achieve a more sustainable world.

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COMPARATIVE LIFE CYCLE ASSESSMENT OF THE ELECTRIC AND HYDROGEN VEHICLES

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Abstract

The transportation sector is one of the primary contributors to the climate change and other detrimental environmental effects. Life cycle assessment is an established method, which provides a quantitative assessment of potential environmental impacts across the life cycle of the vehicle. This study aims to determine total environmental impacts as well as hotspots which contribute significantly to impacts, utilizing modern software and relevant data repositories.

Introduction

Energy consumption has been increasing gradually on the global scale since the beginning of the industrial revolution at the end of the 19th century. The transportation sector has always been the most significant contributor regarding the Greenhouse Gas (GHG) emissions and climate change because it is still almost solely dependent on the fossil fuels. Transportation consumes more than 60% of the extracted oil resources in the world, producing 23% of the carbon dioxide emissions (Van der Hoeven 2014) and utilizing 28% of the final energy supply worldwide (Bicer and Dincer 2017). Furthermore, another major contributor – power generation sector is also heavily dependent on the fossil fuels like coal and natural gas, especially in the developing countries (IEA 2017). Steady growth in both industries has resulted in the continuous detrimental effects on the global environment and human health. Therefore, the substantial necessity for more sustainable and environmentally friendly solutions exists, and a serious effort has been put lately into the development of the appropriate technologies. The latest achievements are represented by battery and fuel cell electric vehicles, hybrid vehicles, and internal combustion engine vehicles utilizing alternative fuels like methanol and next-generation biofuels (Sandy Thomas 2009). Battery electric vehicles, alongside with the hydrogen fuel cell ones are probably the most promising pathways in the future development of the transportation sector, as functional cars utilizing these technologies already entered the market and are serially produced by major manufacturers, like Toyota and Tesla (Wilberforce *et al.* 2017).
Life cycle assessment (LCA) is an established method that can be used to examine potential environmental impacts of the chosen system (or process/product). Full lifecycle or so-called cradle-to-grave approach consists of several stages, including raw material acquisition, production, use, end-of-life treatment, recycling and final disposal (International Standard Organization 2006). Key factors that affect the quality of any LCA study in regard of the vehicles environmental performance include uncertainty of the data, annual vehicle mileage, driving pattern and material recycling rate (Ma *et al.* 2012).

The objective of this study is to compare battery electric and hydrogen fuel cell vehicles regarding potential environmental impacts, identify hotspots and elaborate recommendations addressed to the interested parties.

Materials and Methods

Existing studies in this area have been conducted only recently, and further research is still required to achieve a better understanding of all processes and potential effects associated with the alternative vehicle manufacturing industry. Most notable papers include LCA of hydrogen and gasoline vehicles (Granovskii *et al.* 2006), LCA of the hydrogen and electric

vehicles in Italy (Bartolozzi *et al.* 2013), LCA of hydrogen vehicles in Canada (Ahmadi and Kjeang 2015), LCA of battery and fuel cell vehicles using a well-to-wheel analysis (Li *et al.* 2016) and a few others (Hacatoglu *et al.* 2012; Archsmith *et al.* 2015; Zhao and Tatari 2015). This project will follow international LCA standards and ISO 14044 (International Standard Organization 2006) in particular, which comprises mandatory requirements and provides necessary guidelines. Standard LCA study must include four main phases, namely:

Goal and Scope
The goal of this study is to compare potential environmental impacts of electric and hydrogen vehicles, identify hotspots and help decision makers to choose optimal solutions.

The functional unit is chosen to be 1 km traveled by the vehicle, averaged over the assumed lifetime of the car.

The scope of this study includes "cradle-to-grave" system boundary (entire life cycle from raw material acquisition to end-of-life and recycling, including different electricity and hydrogen production scenarios, with both average European and Irish specific values).

System boundary is presented in Figure 1, given below, and is the graphical representation of the primary LCA stages with the associated inputs (raw materials and energy) and outputs (gaseous, liquid and solid emissions).

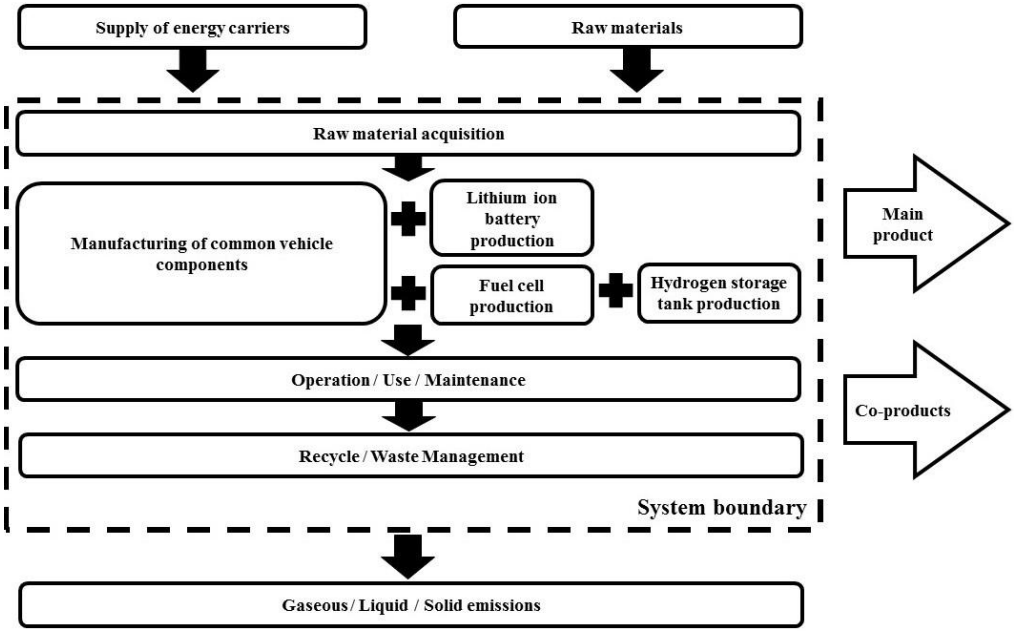

Figure 1. System boundary

Life Cycle Inventory
LCA model building and balance calculations will be performed in the GaBi Education Software. Foreground and background data will be collected from the EcoInvent 3 Database (Ecoinvent 2013), supplemented by the inbuilt data sources provided by the software.

Life Cycle Impact Assessment
The chosen impact assessment method for this study is the CML 2002, developed by the Institute of Environmental Sciences, Leiden University, Netherlands (Universiteit Leiden 2015). CML 2002 is an impact assessment method which restricts quantitative modeling to early stages in the cause-effect chain to limit uncertainties. Results are grouped into midpoint categories according to conventional mechanisms (e.g., Global Warming Potential) or commonly accepted groupings (e.g., ecotoxicity). Table 1, given below, illustrates impact

categories within the method. Results of this study will be expressed regarding this impact categories, scaled to the chosen functional unit.

Table 1. CML 2002 impact categories (European Commission - Joint Research Centre - Institute for Environment and Sustainability 2010)

Environmental impact categories	Unit
Abiotic Resource Depletion (ARD)	kg/year
Global Warming Potential (GWP)	kg CO_2 eq.
Stratospheric Ozone Depletion Potential (ODP)	kg CFC-11 eq.
Photochemical Oxidation Potential (POCP)	kg. C_2H_4 eq.
Acidification Potential (ACP)	kg. SO_2 eq.
Eutrophication Potential (EUP)	kg. PO_4 eq.
Fresh-water Aquatic Ecotoxicity Potential (FAETP)	kg 1.4-DCB eq.
Marine Aquatic Ecotoxicity Potential (MAETP)	kg 1.4-DCB eq.
Terrestrial Ecotoxicity Potential (TETP)	kg 1.4-DCB eq.
Human Toxicity Potential (HTP)	kg 1.4-DCB eq.

Interpretation
Comparisons between battery electric and hydrogen fuel cell vehicles will be performed regarding potential environmental effects and resource consumption. This phase will also include sensitivity analysis on significant parameters, like vehicle mass and operational lifetime, as well as an assessment of data uncertainty and evaluation of the study limitations.

Results and Discussion

This study is still in its early stages, specifically under the data collection phase. Appropriate data acquisition and associated data quality are primary concerns in any LCA study, and rigorous data management plan is required to achieve meaningful results. Expected outcomes will potentially allow to identify environmental hotspots throughout the lifecycle of the both studied vehicle types and help decision-makers in industry, government or non-government organizations to define most suitable solutions.

Conclusion

With increasing vehicle utilization in many countries around the world and limited reserves of the traditional transport fuels, the search for suitable alternatives and development of the innovative approaches to powering vehicles is a necessity. Another sustainability issues associated with the transportation sector like air pollution, global warming and ozone layer depletion caused by the exhaust emissions and during the vehicle manufacture phase also require an adequate response.

Current achievements in both electric vehicle and hydrogen fuel cell technologies provide a promising solution for the problem. This coupled with production of hydrogen from clean, renewable sources such as wind, or solar energy can potentially lead to a better environment for the humanity. Life cycle assessment is an appropriate tool, which provides quantitative, transparent and scientifically valid results, especially when applied to large-scale industrial processes such as vehicle manufacturing and utilization. The results of this study will highlight the critical differences between the two studied types of the vehicles regarding environmental performance and help to increase understanding of the possible issues, that may arise during the transition from the traditional to alternative transportation technologies.

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Ciara Beausang, BSc, MSc

Project Title: Modelling the valorisation options for agri-food waste streams in Ireland

Project Supervisor: Dr Fionnuala Murphy

Abstract

Valorising agri-food waste presents several challenges which need to be addressed in future sustainable value chains. Agri-food waste streams differ from traditional supply chains due to seasonal availability, higher moisture content, low density and high perishability. These challenges have implications for the design, scale and location of future technologies in the bioeconomy. The aim of this research is to examine the potential use of agri-food waste from horticulture in anaerobic digestion, which is currently underutilised in the Irish bioeconomy. Frequently biomass and bioenergy assessments apply a 'top-down' approach; there are few examples of the introduction of bioenergy being driven by the availability of biomass. This research will attempt to fill a gap in the literature by examining a specific waste stream and will assess the feasibility of putting this waste stream to a higher value use in centralised anaerobic digestion. The potential of agri-food waste streams for anaerobic digestion in Ireland have been examined previously, however the focus has been waste streams from livestock production, industrial food production and household organic waste; waste from horticulture has not yet been investigated. A regional case study will determine the geographic distribution, temporal variability and total quantities of horticulture waste in North County Dublin and assess suitability for anaerobic digestion. The data will be mapped to develop a GIS model of waste availability to assess supply and demand scenarios in the region. To assess the sustainability of valorisation with respect to the current management of agri-food waste, Life Cycle Assessment (LCA) will be conducted. This research will help to increase resource efficiency and promote innovation through high value uses of feedstock in the Irish horticulture sector.

FATS, OILS & GREASE (FOG) WASTE MONITORING IN SEWER NETWORKS USING SENSOR TECHNOLOGY

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Abstract

Sewer blockages from fats, oil and grease (FOG) waste is becoming a major problem for cities and around the world due to the increasing populations and the changing diets of residents which leads to more FOG waste entering the sewer networks. Currently there are few strategies in place to prevent the build-ups before they become an issue. Using sensors at known hotspots for blockages could prove a successful method, although this study is still at an early stage of development.

Introduction

FOG waste comes from a variety of sources including food waste and sanitary items from households, along with residues from food service establishments and food processing factories (Wallace *et al*. 2017). It was believed that FOG waste was formed in sewer networks simply due to the cooling of frying oils once they reach the colder sewer networks, but more recent research has indicated that FOG deposits are more accurately composed of metallic soaps due to a saponification process involving calcium and free fatty acids (Williams *et al.* 2012). This combined with sanitary items that are flushed down toilets such as flushable wipes, diapers, condoms etc. can lead to the creation of 'fatbergs' that can block entire sewer networks. This can lead to sanitary overflows - which can pose health hazards – and also increase costs and manhours (Mattson *et al*, 2014).

FOG waste has become a major issue in big cities in recent years and the term 'fatberg' was coined by media outlets to explain these sewer blockages. Outlets such as the BBC, USA Today and National Geographic have all produced articles on fatbergs and the problems they have been causing in major cities throughout the world (BBC 2017; Onyanga-Omara 2017; Engelhaupt 2017). There has been a FOG prevention programme in Ireland that was launched by Dublin City Council in 2008. The programme has been largely successful and has seen a reduction in the number of blockages caused by FOG build-ups (Gibbons *et al.* 2015).

This study is in collaboration with the Science Foundation Ireland funded Connect Centre and their Pervasive Nation project which is the testbed for Irelands 'Internet of Things' (IOT). Gartner Inc. estimated that there were 8.4 billion devices connected through the Internet of Things in 2017 (Van Der Muelen, 2017). The IoT has huge implications for our society as it can enable faster and better broadband capabilities through 5G connections. The millions of devices connected along with the 5G capabilities can enable companies to meet market demand for wireless services to enhance economic and social development (Li *et al*, 2018).

The objective of this study is to determine if sensor technology has the potential to be used to predict and prevent sewer blockages from fats, oils and grease waste.

Materials and Methods

Experimental Design

This experiment requires that sensors be placed inside the UCD campus sewer positioned directly above the wastewater to ensure accurate readings. The sensors are supported by a bracket which is placed well below the manhole cover. The bracket ensures the sensors cannot be disturbed when the manhole lid is removed or by anything underneath.

Sensors

There are two sensors used for this experiment, a Kotahi Level Monitor which is recording the liquid level, and a Sagemcom Siconia PN1 which can record the pressure, temperature and humidity. Both sensors were provided by the Connect Centre in Trinity College Dublin as their research has a focus on IoT applications through the Pervasive Nation project. The level sensor has a data frequency of 1 minute while the Sagemcom sensor has a data frequency of 15 minutes. The devices are located underneath the manhole cover roughly 1.5 metres above the wastewater. Both sensors have lithium cell batteries that will last the duration of the experiment (five months).

The sensors are feeding data back through the Internet of Things network onto a webpage that is run by Pervasive Nation; this allows the user access to the results in either raw data format or in graph format. This webpage can be accessed by all types of devices – including mobile – as long as they have an internet connection.

Results and Discussion

Results for the experiment so far have been limited and show some fluctuations. A sample of the results so far can be seen below in Figure 1 and Figure 2. Figure 1 displays the liquid level results for a fixed period between Feb 21st and March 2nd 2018, and Figure 2 shows the temperature results for the same period.

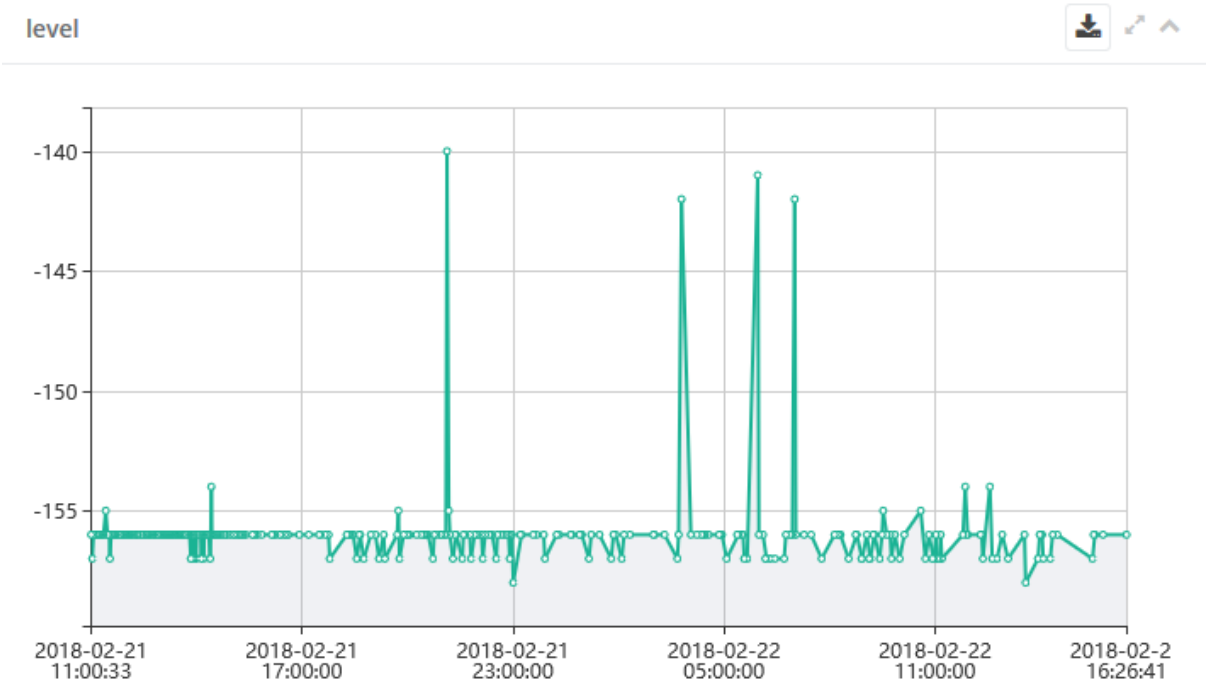

Figure 1. A screenshot of liquid level results for the 21st February – 22nd February.

The results for the liquid level sensors can indicate that there are issues with the setup at the present time, but they also show signs that the sensor is working as required as the level rises and drops by 2 cm at peak hours when the flow of the waste water is at its highest (Figure 2).

The Sagemcom sensor has been feeding back the most reliable data so far as the data is consistent over different days in what it is reading.

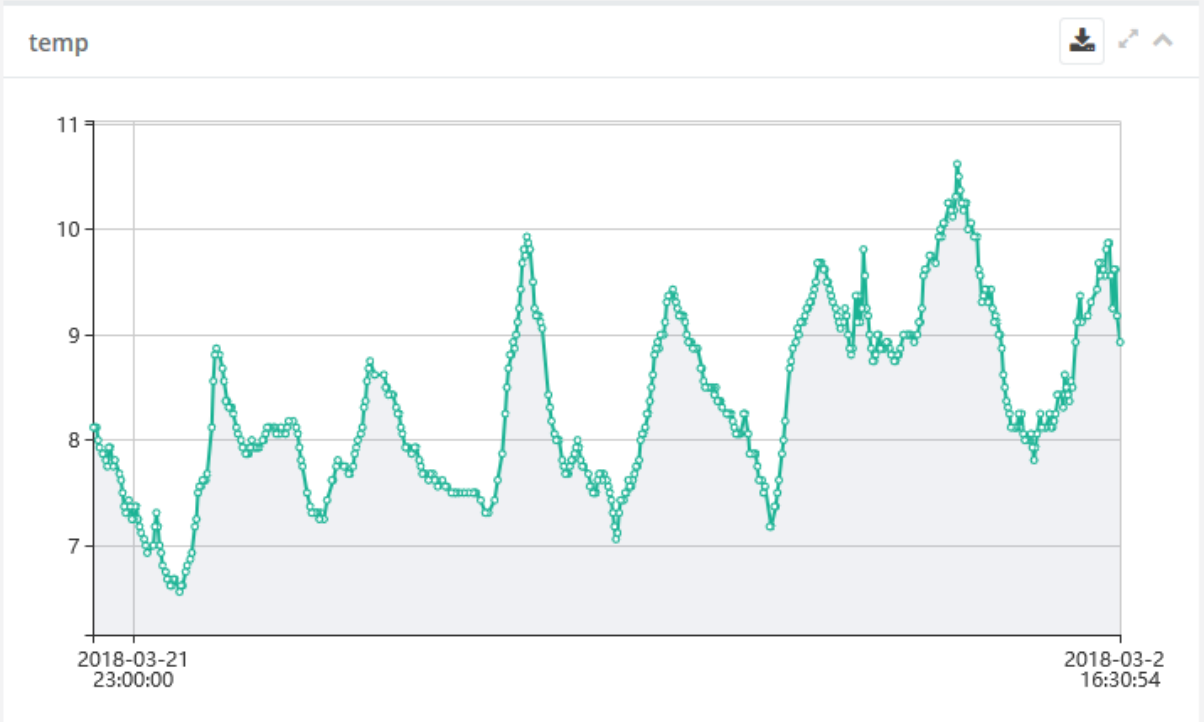

Figure 2. A screenshot of temperature results for the period 21st March – 28th March.

Conclusions

The data so far has been difficult to decipher due to commissioning issues, but the experiment will continue to run and adjustments will be made to ensure the sensors are operational and feeding back data at all times. Based on what has been done so far, it is difficult to determine if theses specific types and models of sensors would be applicable in predicting sewer blockages in cities. From the data gathered, the sensors can tell when the wastewater levels are rising and falling as is seen during peak hours and if it can correctly sense this, then it should be able to tell when there is a blockage and where water levels are rising as a result.

Acknowledgments

This publication has emanated from research conducted with the financial support of the Irish Research Council. The authors would also like to thank the Connect Centre in Trinity College Dublin for the use of the sensors throughout this experiment. The support of a Fulbright TechImpact Award to Dr Tom Curran on this research topic is also acknowledged.

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A SIMPLE ALGORITHM FOR GREEN AREA INDEX

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Abstract

This study aims to develop a simple algorithm for detecting green area index. Cress will be used as a primary research object. Through the analysis of the collected images, an accurate as it is possible algorithm will be proposed. This algorithm will provide the methodological and theoretical basis for the development of future crop remote sensing technology. After further improvements, this method could be optimized and applied to the drone data processing steps in crop remote sensing.

Introduction

Global climate change along with the soil and water pollution has a significant impact on the agriculture production. At the same time, there has been a dramatic increase in global population over the past century which has added tremendous pressure on agricultural production. Without a sufficiently effective intelligent agricultural system, global food shortage is possible in the future. The intelligent agricultural system can help monitor the status and health of the crop and respond to the results in time which will ensure appropriate supply of nutrients, pesticides, and water. Under the monitoring of the intelligent agricultural system, the crop can be kept in the optimal state during the cultivation phase. It can help agriculture industry to create more economic benefits while using limited resources. As a novelty approach in the development of the intelligent agricultural systems, crop optimization through sensing, understanding, and visualization will play an essential role in the future.

Unmanned aerial vehicles (UAV) have been widely used in crop remote sensing and precision agriculture in many countries (Zhang and Kovacs 2012; Huang *et al.* 2013; Shahbazi *et al.* 2014). The algorithm for green area index can provide the methodological basis for crop remote sensing and unmanned aerial vehicle data processing. Standardized and accurate image analysis method and various green area indexes could be calculated through the utilization of this algorithm. Through different indexes and evaluation methods, the holistic cultivation status and health status of the crop could be predicted, potentially improving the efficiency of cultivation. If this algorithm is applied to the large-scale agricultural production system, forecasts and optimized business decisions can be obtained, ensuring that the profits of agricultural production are maximized, and the use of resources is minimized. There is currently not much research in this area. Most studies are limited to the calculation of specific indexes and segmentation methods. There are also some studies on the specific characteristics of a crop. The scope of this kind of study is limited and cannot be widely used in case of other crops and situations.

The objective of this study is to provide the theoretical and methodological framework for agricultural remote sensing and drone data processing in the intelligent agricultural system by developing a simple algorithm for green area index in agricultural production.

Materials and Methods

Materials
Cress is grown indoor by grid growing as a research subject. The structure of cress is simple enough for preliminary study so that the image of cress is concise.

Equipment
Laboratory oven, DSLR camera with a prime lens (Canon EOS 1300D) and tripod (Velbon EX-630).

Image collection and biomass measurement
The image collection method for this study is to photograph the cress in different conditions during the cultivation process. In the process of image collection, the fixed focal length of the prime lens is used to reduce the distortion of the image and maintain the same quality of the image. In the photographing process, the shutter, aperture and center-weighted average metering of the DSLR camera are used in combination to obtain an image with the same exposure value. During shooting, the camera should be placed horizontally to cress to minimize geometric image distortion. The collection of images is mainly for the measurement of green area index (GAI) and leaf area index (LAI). In the process of image collection, to evaluate the GAI index, the steps are to take the leaves off and lie them flat and take pictures of leaves. The fundamental principle of the image collection for LAI is to take pictures of a canopy at single (Liu and Pattey 2010; Ryu *et al.* 2012; Liu *et al.* 2013) or multiple shooting angles (Leblanc *et al.* 2005; Demarez *et al.* 2008; Leblanc and Fournier 2014) The collected images will be segmented into leaf area and background to get LAI result.

In the measurement of leaf area index, the structure of cress is three-dimensional. The vertical projection of plant is smaller than the leaf area index. The effect of the three-dimensional structure of the leaves and the overlapped leaves on the LAI index need to be eliminated. The leaf structure of cress is simple, so in the preliminary experiment, there is no need to consider the overlap of the leaves. In further studies, the overlapping of the leaves needs to be discussed so that the experimental results can be applied to actual operations. Pocket LAI is a mobile application for leaf area index (LAI) estimates. In this study, it will be used to make preliminary LAI predictions. In the process of image collection, detailed image collection methods need to be considered to develop accurate LAI measurement methods.

During the image collection phase, various noises in the image should be avoided or eliminated as much as possible. The soil background, the dead leaf, stone and anything else which may affect the image processing should be considered. Shadow is a factor which has the most significant influence on the image quality in the image collection phase. Due to the different angles of light, the area of the shadows is different. Shadows have different effects on image quality under different lighting conditions. The shadow in the image should be distinguished and eliminated. The use of a flash and a diffuser can efficiently remove shadows during the photographing process.

Biomass detection is an essential factor in the green area index. Because image collection can provide data such as the color and leaf area of cress, the evaluation of the green area index requires direct measurement of the biomass to assist in the accuracy of the algorithm. To measure the biomass, the stems and leaves of cress need to be separated and weighed for both wet and dry weight. Combining the green area index and leaf area index with biomass, the mass of cress per unit area could be calculated.

Image processing

The image processing problem is the focus of this research. The green pixels are the most critical research object of this study. The ImageJ software will be used to analyze the green pixels in the image of cress. It can calculate area and pixel value statistics of user-defined selections. Spatial calibration is available to provide real world dimensional measurements in units such as millimeters. With the help of this image processing program, the green pixel data in the image would be extracted and evaluated. There are three main steps in the process of image processing. The first step is to normalize the image to reduce the geometric distortion of the image. However, because a prime lens will be used in the photographing procedure, the geometrical distortion of the image will be minimized. In the initial stages of the study, no particular corrective actions are required. The second step is to remove the noise. The noise of image needs to be eliminated for accuracy consideration. During the image processing stage, removing noise from the image such as erosion method could help in noise removing. The third part is segmentation. In the image of cress, the green pixels are segmented and extracted. This step extracts the green pixels data in the image and converts it into biomass, green area, and leaf area estimation. The accuracy of the segmentation method determines the quality of the study results.

Data analysis

The green pixel data obtained at the image processing stage indicates the green area index and the Leaf area index. Combining the data of GAI and LAI with biomass data can make a general assessment of the growth of cress. Other indexes like normalized difference vegetation index, enhanced vegetation index and soil-adjusted vegetation index will also be discussed for the accuracy of the algorithm.

Results and Discussion

The primary aim of this paper is to develop a simple algorithm for green area index with solutions for noise, shadow, and segmentation of the image. Based on this study and any other fundamental research, further crop remote sensing research could be developed.

The accuracy of the algorithm determines the accuracy of green area index. The accuracy of the algorithm has many influencing factors. The cultivation method of cress, the rational use of equipment and materials in the process of image collection, the normalization and consistency of image collection, the rationality of image processing and the method of data analysis all influence the accuracy and feasibility of the simple algorithm. This simple algorithm for the green region needs to be considered in conjunction with the species of the subject. Although the evaluation of various indices can be obtained through direct analysis, accurately predicting the growth status of the subjects requires the combination of leaf growth characteristics of different experimental subjects.

Conclusion

The simple algorithm of the green area index is rooted in the subject of crop remote sensing and unmanned aerial vehicle (UAV) data processing. This algorithm provides the most basic and preliminary theoretical basis for the intelligent agricultural system. Using this simple algorithm, the holistic cultivation status, health status of crop and production forecasts could be predicted in the intelligent agricultural system to get maximized profit and minimized resource consumption. Through the development of the accuracy of this algorithm, a comprehensive analysis of a wide range of crop images and close-up images of crops can accurately detect the cultivation status and health status of crops and then guide agricultural decision-making and agricultural planning. As a

conjecture, this algorithm can also be applied to the monitoring of standardized production of large-scale agricultural production such as tea.

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AMMONIAN2K: PRELIMINARY MONITORING OF AMBIENT AMMONIA ON NATURA 2000 SITES IN IRELAND

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Abstract

Ammonia is one of the five air pollutants set under the National Emissions Ceilings Directive (2016/2284/EU) which targets emission reductions for 2020 and 2030 of 1% and 5% respectively based on 2005 figures. In Ireland, over 100 Kilotonnes of ammonia is emitted annually, of which agriculture is responsible for 98%. Ammonia can negatively impact the environment through both eutrophication and acidification. Critical levels have been set internationally for lichens and mosses (1 µg/m3) and higher plants (3 µg/m^3). A critical level refers to a concentration in the air above which negative impacts are likely to be observed. Sensitive areas such as Natura 2000 sites which are internationally designated areas of ecological importance can be particularly at risk from elevated ammonia concentration levels. This research is taking place over a 12-month period with provisional results available for the month of August in this paper. These have shown that many sites appear to lie between the critical levels of 1 µg/m^3 and 3 µg/m^3 of ammonia concentrations in the atmosphere, while midland bogs regularly exceed both critical levels. on sites where slurry was spread, notably higher concentrations of ammonia were observed.

Introduction

Currently there is a lack of data on ammonia concentration levels in the Irish atmosphere with only two previous studies being conducted by the EPA in 1999 (Farrell, 1999) and in 2013-2014 (Doyle *et al.* 2014). In the UK ammonia concentrations have been monitored since 1996 (UKEAP 2018). As concerns over global warming and biodiversity grow so does the focus on nitrogenous emissions into the atmosphere, in Ireland ammonia is a major nitrogenous pollutant. This study looks to improve on previous studies in building a database of ammonia concentrations in Ireland by monitoring of precise ammonia concentrations for selected Natura 2000 sites. Under the NEC Directive (2016/2284/EU) all EU member states are obliged to monitor atmospheric ammonia concentrations at risk sensitive sites. This study is the first to monitor ammonia concentrations on Natura 2000 sites in Ireland. Natura 2000 sites are sensitive areas of international ecological importance they are protected by directives such as the habitats directive (92/43/EEC) and birds directive (2009/147/EC), currently around 75% of Natura 2000 sites in Ireland are deemed to be in poor condition, therefore many improvements are needed (O'Connor 2015). Monitoring ammonia concentrations at these sites can give authorities information on the potential impacts that may be caused from elevated ammonia levels such as acidification and eutrophication. The higher the recorded ammonia level the more negative impacts may be observed any reading below the 1 µg/m^3 critical level is likely to have to have no negative impacts on the surrounding environment (Wang *et al.* 2015).

This project is currently monitoring 12 Natura 2000 sites within the Republic of Ireland. An additional site in Lough Nevar, Northern Ireland is being monitored for cross calibration purposes with the monitoring network in the United Kingdom further information can be found on the CEH website (CEH 2017).

The objective of this study is to determine the atmospheric ammonia concentrations on 12 Natura 2000 sites within the Republic of Ireland.

Materials and Methods

Concentrations are recorded using ALPHA (Adapted Low-cost Passive High Absorption) samplers which are provided by the Centre of Ecology and Hydrology (CEH) which are prepared monthly in UCD and posted out to National Parks and Wildlife Services (NPWS) staff who exchange the samplers on site. These are then returned to UCD every month for analysis. The use of the ALPHA samplers is the Best Available Technique (BAT) available for this study. The ALPHA samplers which are designed by the Centre for Ecology and Hydrology (CEH) who also operate the site in Lough Nevar which as previously stated is being used for cross calibration.

Selection of sites

Under the National Emissions Ceilings directive sites for monitoring should be selected based on risk assessment (Sutton *et al.* 2004). As this is a provisional monitoring program trialling cooperation with the NPWS staff, sites were selected based on NPWS staff availability. The Natura 2000 sites monitored host a range of habitats from blanket bogs to raised bogs and grasslands this allowed for a relatively broad range of Natura 2000 habitat types to be covered despite a small sample size. The list of sites is displayed in Table 1. An additional site in Lough Nevar, Co. Fermanagh was also used for cross calibration with the CEH in the UK.

Site set up

At each site a pole was driven into the ground to provide support for the platform for sampling, a plate was attached to this pole at a height of 1.5 m. Three ALPHA samplers will be attached to the underside of this plate using Velcro. The plate acts as a cover from rain and wind, it is also the recommended height for monitoring atmospheric ammonia (Tang *et al.* 2017).

Table 1. List of site names, location and descriptions.

Site name	County	Site description
Wicklow Mountains SAC	Wicklow	Blanket bog
Blackwater Valley	Cork	Fresh water pearl mussel
Kilconney Bog	Cavan	Raised bog
Wexford Wildfowl Reserve	Wexford	Wildfowl
Raheenmore Bog	Offaly	Raised bog
Spahill and Clomantagh Hill SAC	Kilkenny	Semi natural dry grassland
Lough Nevar	Fermanagh	Cross calibration
Bricklieve Mountains & Keishcorran SAC	Sligo	Turloughs
Ardgullion	Roscommon	Raised bog
Brown Bog	Longford	Raised bog
Garriskill (approximate)	Westmeath	Raised bog
Lough Lene	Westmeath	Crayfish
Scragh bog	Westmeath	Feather moss

Lab work

To prepare the filter papers used in the ALPHA samplers, 6 g of citric acid was dissolved in 50 ml of methanol. A pipette was used to add 55 microliters of the citric acid solution to each filter paper. These were subsequently placed in a vacuum chamber for four minutes to dry rapidly. The ALPHA samplers are then assembled as per figure 1, following a thorough wash to ensure no contamination is present from the previous exposure. These samplers are then placed in an air tight bag before being packaged and dispatched to each of the 13 monitoring sites. Four ALPHA samplers are sent to each site with three being placed out on the site and one being kept in the air tight bag as a blank, this accounts for any possible contamination during transport. Four additional samples are kept in the lab as laboratory controls.

ALPHA samplers are sent out to each of the 13 sites and returned to UCD each month. Once returned the filter papers are then soaked in 3 ml deionised water for an hour before extracting 200 microliters

of the deionised water and dispensing it into new tube. 4 ml of salicylate reagent and 1 ml hypochlorite reagent are then added and mixed well before being left to settle for 20 minutes (Tang *et al.* 2017). A Hach Lange spectrophotometer was used to read the absorbance levels of each sample this is done by placing 2.5 ml of the solution in a cuvette and placing it in the spectrophotometer. A cuvette filled with deionised water is placed into the spectrophotometer before each sample to re-zero. Known concentration absorbance readings were recorded for each batch these known concentrations were 10ppm, 1ppm, 0.1ppm and 0ppm. This lab procedure is based on previous work carried in 1996 (Willis et al. 1996).

Data Analysis

All results are calculated using Excel. The formula shown in Figure 2 is that of the line of best fit from a calibration curve produced using absorbance readings of known concentration levels. The absorbance readings are input to this formula which then allows the ammonia concentration to be solved.

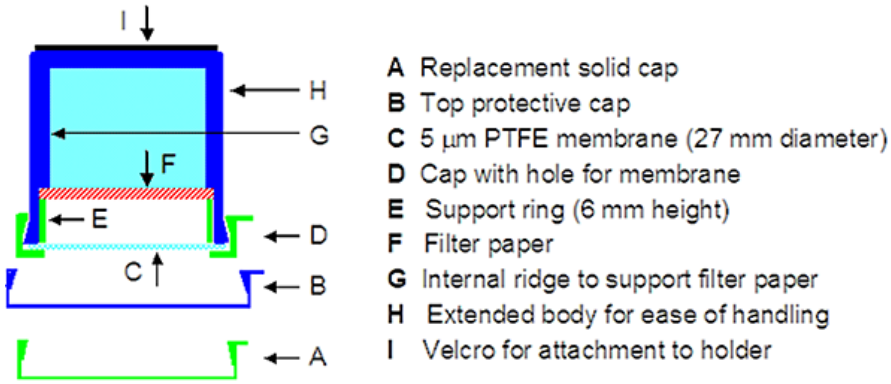

Figure 1. ALPHA sampler components (CEH user guide 2017).

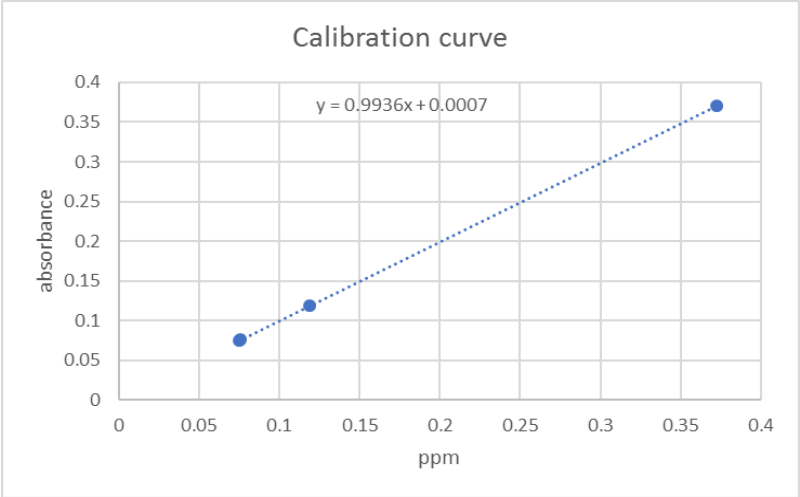

Figure 2. Formula used from line of best fit to find ammonia concentration.

Results and Discussion

The preliminary results for August are displayed for each site in Table 2. There is a notable high reading in Lough Lene; however this was expected as it was noted slurry spreading occurred during this trial period. It is known that slurry spreading can release large amounts of ammonia via volatilisation, trailing shoe can reduce ammonia emissions by as much as 30% compared to splash plate slurry spreading (Misselbrook *et al.* 2002). The lowest ammonia concentration reading was in the Wicklow Mountains where intensive agriculture is not as common as in other parts of the country due to the mountainous terrain. Nine sites were above the critical level of 1 µg/m^3 it would be expected to see negative impacts on lichens at these sites such as poor growth performance and a shift in species (Doyle *et al.* 2017). Only two sites had recorded levels of less than 1 µg/m^3.

Table 2. Preliminary results for August.

Site name	µg/m^3
Wicklow Mountains SAC	0.4
Kilconney Bog	2.2
Wexford Wildfowl Reserve	1.4
Raheenmore Bog	3.1
Spahill and Clomantagh Hill SAC	1.8
Enniskillen	0.5
Ardgullion	1.3
Brown Bog	2.1
Garriskill	1.3
Lough Lene	17.1
Scragh Bog	1.8

Conclusions

In order to carry out full in-depth research study on ammonia concentrations on sensitive sites in Ireland full time dedicated staff are required as currently this study is time limited. With a dedicated staff person replacing and analysing samplers, it is estimated as many as four times the amount of sites could be monitored. It is also worth noting that agriculture does have an effect on ammonia concentrations as those sites located within intensive farming areas appear to have higher concentrations than those sites in remote areas. The results to date have indicated that the majority of sites lie above the 1 µg/m^3 critical level so according to this negative impacts are already occurring to lichens and mosses on these sites.

Acknowledgements

The authors would like to thank the NPWS staff who kindly volunteered to switch ALPHA samplers each month; without them this project would not have been possible. Thanks also to the National Wildlife Parks and Wildlife Services and the Environmental Protection Agency for funding and support of this study as part of the AmmoniaN2k project (https://www.ucd.ie/ammonian2k/).

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ADSORPTION OF ORGANIC DYES IN WATER BY ALUMINIUM OXIDE AND A RESEARCH ON THE PROCESS OF ADSORBENT REGENERATION

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Abstract

Given the worldwide scope of water bodies, water contamination affects the entire biosphere of plants and organisms, which can lead to environmental degradation of aquatic ecosystems and public health problems. With the growing pace of industrialization, there are more than 10,000 types of dyes used as coloring agents. The discharge of effluents containing persistent and toxic dyes has become a widely discussed concern. Till now, there are several techniques utilized to deal with organic dyes in water and aluminum oxide has been proven to be a successful and effective adsorbent. Different kinds of aluminum oxide prepared under different temperature will be applied to absorb organic dyes in water, and absorbents will be regenerated with sodium hydroxide solution and hydrochloric acid solution. Regenerated aluminum oxide will undergo adsorption experiments again. The purpose is to find theoretical basis for adsorbent regeneration and best choice for reality application. For statistic, visible spectroscopy is utilized to quantify the dye concentration after treatment directly.

Introduction

Aluminum oxide is a chemical compound of aluminum and oxygen with the formula Al_2O_3. All kinds of aluminum oxide have been applied widely in different areas, for example, structural ceramic materials, aluminum alloys, pharmaceutical, integrated circuit plate, laser materials, adsorbents, catalyst and catalyst support (Al-Abadleh and Grassian, 2003). Aluminum oxide has been proved to be a successful absorbent for dealing with contamination in water, because it is a porous solid material and has great specific surface area (BET) (Mohan and Pittman, 2007). For its formula Al_2O_3, aluminum oxide is a kind of simple oxide. However, there are 9 types of crystalline structure, and is conventional to denote these forms by the reek letters α, β, γ, δ, η, κ, θ, ρ, and χ (Kulinkin *et al.* 2000). Not only in different kinds of crystalline structure, but also in the same crystalline structure, there are huge difference between the macroscopic and microscopic structural properties (for instance, density, pore volume, pore size distribution and specific surface area). Also, varieties in preparation methods cause difference. The diversity of crystalline structures determines its broad area of application on the one hand, but makes difficulty for mastering its regularity. **The objective of this study was to compare the adsorption capacity of different alumina oxide, choose the alumina oxide with best performance, and characterize its feature.**

Materials and Methods

This subject mainly concentrates on the adsorption of organic dyes in water by different kinds of aluminum oxide calcinated under different temperature, specific details are shown below:

1. Calcinate the boehmite under different temperatures to prepare aluminum oxide

absorbents,which is used to absorb organic dyes. These absorbents will be characterized by XRD, BET and HR-TEM.

2. Calculate the adsorption capacity of different aluminum oxide.
3. Conduct regeneration experiments of used aluminum oxide and absorb organic dyes in water by regenerated aluminum oxide, in the aim of exploring the effect of temperature on regeneration.

1. Preparation of aluminum oxide

These experiments aim to investigate the performance of Al_2O_3 calcinated under different temperatures for 4 hours. Temperatures are chosen to be: 400 ℃, 500 ℃, 600 ℃, 650 ℃, 700 ℃, 750 ℃, 800 ℃, 850 ℃, 900 ℃, 1000 ℃.

2. Saturated adsorption experiment

Measure 100 ml of organic dye solution (concentration is 100.0mg/L), and move it to 300 ml beaker. Add 500 mg Al_2O_3 to it, stir the solution for 24 hours, then filter it: (a) Residue of Al_2O_3 is heated under 80 degrees for 3 hours, and saved for further study; (b) Measure the luminousness of solution, so the efficiency and quantity of absorbed organic dyes can be figured out (visible spectroscopy is also used to quantify the dye concentration after treatment directly).

3. Regeneration of Al_2O_3

Put the residue of Al_2O_3 into a breaker, add 10 ml of NaOH solution (concentration is 0.1 mol/L), stir the solution for 0.5 hours, then filter it. The residue is heated under 80 degrees for 3 hours. The same procedure treated with 10 ml of HCl solution (concentration is 0.1 mol/L), complete the regeneration.

4. Saturated adsorption experiment with regenerated Al2O3

Use regenerated Al_2O_3 to absorb organic dyes, procedures are same with 2.

5. Characterization of Al_2O_3 absorbents

All samples of Al_2O_3 calcinated under different temperatures will be characterized by X-Ray Powder Diffraction, Raman Spectroscopy/Imaging, High Resolution Transmission Electron Microscopy, and UV-visible spectrophotometry.

Results and discussion

Prediction of adsorption value

Table and figure below are from the research I did before, which uses alumina oxide to absorb fluoride.

Table 1: Specific surface area, pore volume and saturation capacity of Lab-X calcinated at different temperature

Samples (Calcining temperature)	Specific surface area (m^2/g)	Pore volume (cm^3/g)	Adsorption capacity (mg/g)
Lab	548.7	1.62	
Lab-400	533.5	1.75	94.35
Lab-500	531.8	1.83	98.27
Lab-600	488.1	1.82	95.21
Lab-650	466.1	1.75	93.17
Lab-700	361.3	1.71	90.54
Lab-750	293.3	1.65	88.39
Lab-800	236.2	1.43	83.49
Lab-850	215.4	1.40	75.17
Lab-900	204.2	1.32	61.32
Lab-1000	150.8	0.87	31.74
Lab-1200	30.2	0.04	1.35

In the laboratory Lab-X samples, Lab-400 is a boehmite that has not completely converted to γ-alumina from the perspective of its crystals. Although its specific surface area is larger than Lab-500, its adsorption capacity is smaller than that of Lab -500; when the calcination temperature ranges from 500 °C to 800 °C, the sample behaves as γ alumina crystal form, Lab-500, Lab-600, Lab-650, Lab-700, Lab-750 and Lab-800 activated alumina adsorbents showed relatively optimal adsorption capacity for fluoride ions. The adsorption efficiency of 0.5 g Lab-500 adsorbent for 100 mL 500mg/L fluoride ion solution reached over 98%; while the calcination temperature was above 850 °C, Lab-X starts to transform from γ-alumina to α-alumina, and the specific surface area drops significantly. The specific surface area of Lab-1200 is only 30.2 m^2/g. The sample has lost the original appearance of flaky folds and sintered into flakes. The structure can hardly adsorb fluoride ion in water, and its adsorption capacity is only 1.35 mg/g.

The performance of absorbing organic dyes may differentiate from fluoride, that is what we will focus on the relationship between crystalline structure and adsorption capacity.

Characterization of Al_2O_3

Take XRD as an example, when the sample was calcined at 400 °C, the peak intensity decreased with respect to sample was not calcinated, and the peak position shifted to the characteristic peak of γ-Al_2O_3, which indicated that the sample calcined at 400 °C was not completely converted to γ-Al_2O_3. It represents this sample located at transformation from boehmite to γ-Al_2O_3; Alumina samples calcined at 500-800°C exhibited characteristic peaks of γ-Al2O3; When calcination temperature reached 850-1000°C, the samples exhibited θ-Al2O3 characteristics near 2θ of 32.89° and 40.05°. Peak, the sample at this time is a

mixture of γ-Al2O3 and θ-Al2O3; when the calcination temperature is 1200°C, the sample exhibits a characteristic peak of α-Al2O3, and the sample has been converted into α-Al2O3 completely.

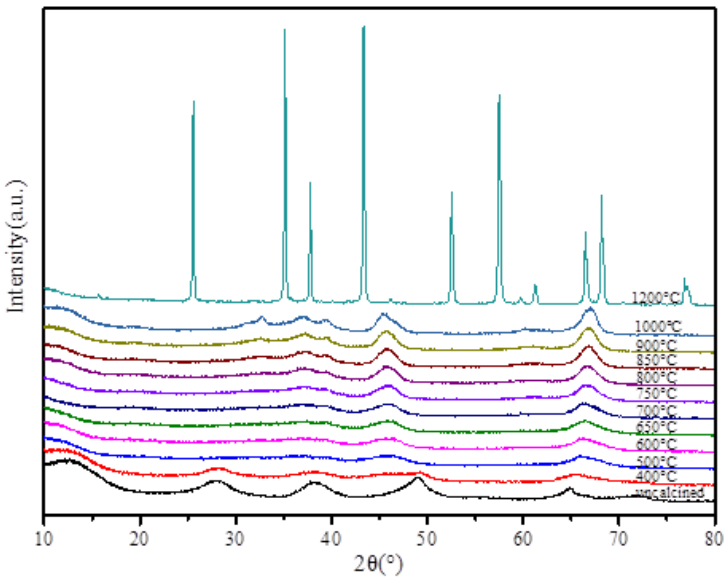

Figure 1: XRD patterns of Al203 absorbents prepared by boehmite calcinated under different temperature

By comparing adsorption capacity of different aluminum oxide calcinated under different temperatures, the difference of adsorption capacity between aluminum oxides with different specific surface area and crystalline structure can be explored, while theoretical guidance will be provided for choosing suitable temperature of calcination. By investigating the process of regeneration of aluminum oxides calcinated under different temperature, acid-alkali resistance of different Al_2O_3 can be explored, while theoretical guidance will be provided for regeneration. The best suitable condition for calcination can be selected and the best aluminum oxide chosen. An absorbent which is able to be utilized for several times and cut down expense.

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Project Title: A risk assessment of the environmental fate of silver nanoparticles through the aquatic environment

Project Leader: Assoc. Prof. Enda Cummins

Abstract

Risks posed by silver nanoparticles released to the environment are poorly understood as environmental concentrations remain uncertain which is an impediment to viable risk assessments. Silver is naturally present in the environment, but the presence of engineered forms (unnatural) of nanosilver (nAg) may cause a toxicity concerns to biological organisms due to uptake and the potential release of ionic silver (Ag^{+}). The objective of this study is to assess the fate and behaviour of nAg in aquatic systems and the potential for these materials to persist in such systems and the risks posed by persisting nAg. In-situ processes of particle dissolution, aggregation and sedimentation where deemed to be the main drivers in the fate and behaviour of nAg in complex aquatic systems. Data pertaining to these processes was collated from literature and through bench scale experimentation to determine the likely persistence of nAg following these in-situ processes. A mass balance model was developed incorporating probability distribution to predict the likely removal of nAg concentrations with two types of stability coatings following each in-situ process over time. Monte Carlo simulation where run with 10,000 iterations using the @Risk 7 software package to account for the uncertainty in the data and variability in the processes. The initial concentration of nAg was calculated using literature modelled and measured values and was presented through a triangular distribution to represent a worst-case scenario for Irish waters with a mean concentration of $4.34E^{-2}$ μg/L. Residual nAg over 168 hrs indicated that concentrations were several orders of magnitude below toxicity levels for aquatic organisms. The in-situ processes incorporated in this model indicated the time dependence required for them to reduce the initial input concentrations of nAg. The presence of stability coatings is likely to inhibit the in-situ processes leading to persisting concentrations of nAg. Water flow is likely to transport nAg to transitional waters over time leading to accumulations in these zones and potentially present a toxicity risk in accumulation hotspots.

Recent Publications

Shevlin, D., O'Brien, N., Cummins, E. (2018) 'Silver engineered nanoparticles in freshwater systems – Likely fate and behaviour through natural attenuation processes', *Science of The Total Environment*. 621C, pp 1033 – 1046.

Felipe Guth, B.Sc., M.Sc.

Project Title: Disease level assessment in crop plots using RGB images and deep learning algorithms

Project Leaders: Prof. Shane Ward and Prof. Kevin McDonnell

Abstract

The assessment of disease levels in crop fields is an important, time consuming task that generally relies on expert knowledge by trained individuals. Image classification in agriculture problems historically has been based on classical machine learning strategies that make use of hand-engineered features in a top of the classification algorithm. This approach tends to produce results with low level of both accuracy and generalization to the relationships classified by the system, due to the nature of the elements having a significant variability. The advent of deep convolutional neural networks has revolutionized the field of machine learning, especially in computer vision tasks. These networks have great resourcefulness of learning and have been applied successfully to image classification and object detection tasks in the last years. The objective of this research was to propose a new method based on using deep learning convolutional neural networks for the task of disease level monitoring. Common RGB images of winter wheat were obtained to derive 5 classes of disease levels presence that could be classified by the system. Disease level tasks performed by experts provided ground truth data for the disease score of the same winter wheat plots were the images were acquired. The results obtained using the testing set over the 5 classes of disease level proposed by the system achieved an overall accuracy of 83%. In the between classes the accuracy varied from 75% on the worst to 92% in the best case. These results have shown the viability of the deep learning approach for disease level monitoring in wheat plots and has also provided evidence that this approach can be derived to applications in other crop types. The main limitation of the proposed work relies on the quantity of data provided. Despite a of data augmentation techniques, the ideal scenario is the one that contains a significant number of unique original images for each class with enough variability to allow the deep net to extract the underlying features that can best characterized each category. The lesser accuracy scores were found in the second (5-9.9% of disease presence) and third (10-19.9% of disease presence). This condition is a consequence of the difficulty in detecting the differences in the inter classes and their differences with the first class as well (0-4.9% of disease infection).

Recent Publications

Guth, F., Ward, S., McDonnell, K. (2016) 'Autonomous Winter Wheat Variety Selection System', *Journal of Advanced Agricultural Technologies (JOAAT)*, 4, 104-110.

Guth, F., Ward, S., McDonnell, K. (2017) 'A Review of Machine Learning Towards Precision Agriculture in Crop Production', *Journal of Environmental Science, Computer Science and Engineering & Technology (JECET)*, 6, 492-510.

Guth, F., Ward, S., McDonnell, K. (2016) 'Crop Disease Detection Through Deep Learning Convolutional Networks', *Manuscript submitted for publication*.

Kathleen Dunne, B.Sc. (Hons.)

Project Title: Prediction of phosphorus sorption capacity in agricultural soils using DRIFT spectroscopy

Project Leaders: Prof. Nick Holden and Dr. Karen Daly

Abstract

Foodwise 2025 set challenging targets in Ireland, to increase agrifood exports by 85 % and the value of primary production by 65 % in the coming decade. Soil health will play an important role in meeting these targets. Soil fertility, is monitored by testing for parameters such as: pH, organic matter, aluminium (Al), iron (Fe) and phosphorus (P) sorption capacity. Soil testing for P is also required under the Nitrates Directive, to protect water quality and prevent the over-use of fertilizers. However, there are disadvantages associated with traditional soil testing methods: they are time-consuming, costly and produce a lot of chemical waste. The objective of this study is to explore the use of infrared diffuse reflectance (DRIFT) spectroscopy as a rapid, cheap and environmentally friendly alternative to traditional soil testing methods. It is hoped that this method will act as a surrogate, specifically, for methods related to P sorption dynamics in soil. To date, this project has used conventional methods to build a laboratory database of sorption parameters. This database is comprised of 225 first horizon Irish Soil Information System (SIS) samples, to a depth of 30 cm. These same samples were ball-milled and scanned on a dual-rage, bench-top, PerkinElmer Spectrum™ 400, in mid infrared (MIR) mode. Absorbance of each sample was read in triplicate. Spectra were exported as '.csv' files, read into R Studio and replicates were averaged for partial least squares regression (PLSR) model development. A modification of the standard batch technique of Nair et al. (1984) was used as a phosphorus sorption isotherm reference method and preliminary MIR calibrations were generated for Langmuir sorption parameters, Xm, the sorption maximum (mg P kg^{-1}) and b, an affinity constant related to binding energy (l mg^{-1}). To date, preliminary prediction results, using PLSR, for the sorption maximum, Xm, have been indicative of a reliable model (calibration $R^2 > 0.7$, RPD > 1.8) and less reliable for the affinity constant, b ($0.55 \leq$ calibration $R^2 \leq 0.65$, $1.5 \leq$ RPD ≤ 1.8). It is hoped these prediction results will be improved, through model optimization using spectral preprocessing and an appropriate validation technique.

J.P. Emmet-Booth, B.Sc. Ag. (Org), M.Sc. Ag.

Project Title: Evaluation of visual soil structure assessment methods for research and management deployment in temperate maritime grassland and arable soils

Project Leader: PD Forristal, O Fenton, N Holden.

Abstract

As humankind begins to comprehend the extent and consequences of global soil degradation, principally caused by soil mismanagement, the race to develop conservation strategies at both policy and practical land management levels intensifies. Visual Soil Evaluation (VSE) techniques are increasingly recognised as important soil quality assessment tools appropriate for both research and sustainable soil management. Many VSE techniques exist internationally and despite varying methodologically, involve the visual, tactile and occasional olfactory assessment of soil properties principally related to soil structure, the latter underpinning overall soil quality. In temperate maritime climates, soil structural degradation is of particular concern, notably by soil compaction. The objective was to develop VSE techniques as tools appropriate for farmer use, to aid real-time soil structure management. The first phase required the development of GrassVESS, a modified version of an existing VSE technique to enhance grassland assessment efficiency. GrassVESS was tested by an operator focus group along with a national survey, which included 30 Irish grassland sites. GrassVESS correlated well with quantitative indicators of soil quality while the incorporated modifications were justified by the operator focus group. The second research phase concerned arable soils. A survey of ten sites across Eastern Ireland allowed conflict between VSE methodology regarding assessment depth to be explored, with the aim of increasing efficiency of assessment in agricultural advisory scenarios. Results indicated that VSE to 40 cm depth was necessary to guide soil management though assessment to 80 cm was required to indicate the extent of management impacts. Finally, the sensitivity of VSE techniques in detecting yield-impacting compaction was investigated using crop trials conducted at the Teagasc Oakpark over two seasons. Graduated levels of experimentally imposed compaction on plots of winter barley (*Hordeum vulgare* L.) in randomized block design were successfully identified by VSE conducted to 40 cm depth which corresponded with quantitative soil measurements. However, VSE diagnoses translated into a yield response only on loam soils and not a sandy soil, though this may have been a result of the short duration of the experiment. Overall, this research confirmed the utility of VSE techniques for temperate maritime grassland and arable soil quality assessment and improved the efficiency of techniques as real-time soil management decision support tools.

Selected Recent Publications

Emmet-Booth, J.P., Forristal, P.D., Fenton, O., Ball, B.C. Holden, N.M. (2016) 'A review of visual soil evaluation techniques for soil structure', *Soil Use & Management*, 32, 623-634.

Emmet-Booth, J.P., Bondi, G., Fenton, O., Forristal, P.D., Jeuken, E., Creamer R.E. Holden, N.M. (2018) 'GrassVESS: a modification of the visual evaluation of soil structure method for grasslands', *Soil Use & Management*, 34, 37-47.

Tenzin Tashi, BE, MSc

Project Title: Process Modeling and Life Cycle Assessment of Skim Milk Powder (SMP)

Project Leader: Prof. Nicholas M Holden

Abstract

Due to the abolishment of the EU milk quota in April 2015, Ireland set a target of a 50% increase in milk production by volume by 2020, which represents about 7.6 billion liters of milk. This has significant implications for the function, efficiency and impact of the dairy processing industry. Mass flow and environmental impact models can be used to provide information about efficiency and impact. Since there is a lack of high resolution empirical data for the energy and water consumption at each unit operation along the production chain, it is necessary to use process modelling of skim milk powder (SMP) production. The objective of this research is to develop a process model for the creation of SMP from raw milk, to use with life cycle assessment. Process design software (SuperPro Desginer V.10) was used to develop a flowsheet process model for each unit operation that will be validated by parameterizing and calibrating the model with the energy and water data collected from different Irish dairy plants. This validated process model will be used to represent SMP production, and mass and energy balance data for the key unit operations such as pasteurization, evaporation, spray drying, and CIP operation will be used as an input data for life cycle assessment by combining with data collected onsite for other activities. Gabi software will be used to for the LCA with the main focus being carbon footprint. It is expected that this research project will explore the reasons behind energy and water consumption variation in different Irish dairy plants manufacturing SMP. Moreover, the hotspots in the process will be identified to guide the dairy processors in reducing greenhouse gas emissions, increasing throughput, reducing cycle time and reducing production costs. Therefore, this research work will assiss Irish dairy processors to move towards more sustainable production of skim milk powder.

Appendix 1

(Research projects in progress which have not been included in the Research Review)

Achata EM, Esquerre CA, O'Donnell CP. NIR - Hyperspectral imaging and chemometrics as a pat tool for the prediction of food powders mixing kinetics (**PhD**). FIRM as administered by the Irish Department of Agriculture, Food and the Marine.

Fahy J and Butler F. Sampling pogrammes for Norovirus in shellfish (**MEngSc**).

Henihan L and O'Donnell C. Development of PAT tools for quality and safety improvement in dairy ingredient manufacture for infant formula (**PhD**). Food Institutional Research Measure (FIRM) administered by the Irish Department of Agriculture, Food and the Marine.

Herron J, Moloney A, Curran T. A preliminary review of management factors affecting nitrous oxide emissions from livestock systems (**PhD**). Teagasc Walsh Fellowship Scheme.

Hunt K, Butler F, Doré B, Keaveney S. An assessment of RT- QPCR accuracy in monitoring infectious norovirus in oyster farms (**PhD**).

Kelleghan D, Lambert D, Curran TP. Identifying below threshold intensive agriculture units in Ireland (**PhD**). STRIVE EPA.

Li F and Butler F. Efficacy of novel thermal and non-thermal processes to reduc e spore numbers within daiy manufacturing processes (**PhD**).

Liu R and Holden N. Greenhouse gas emissions from homogenization for liquid milk production (**PhD**). CSC-UCD Scholarship Scheme.

Panikuttira B and O'Donnell C. Development of process analytical tools for food processing (**PhD**).

Qichen Hao and Butler F. The use of whole genome sequencing to investigate the tempor al and spatial occurrence of microbial pathogens in a dairy processing facility (**PhD**).

Rice P, Holden NM. Formulating a functional unit for dairy production lifecycle assessment considering the financial function of the product (**PhD**). Irish Department of Agriculture, Food and the Marine.

Sharma P, Humphreys J, Holden NM. Intensification or extensification? environmental impacts of Irish dairy farms (**PhD**). Irish Department of Agriculture, Food and the Marine.

Stanley S, Crickley S, Curran T. Impact of european and irish legislation on the design of dairy wastewater treatment processes (**MSc Res**). Irish Research Council Employment Based Postgraduate Scheme in collaboration with WEW Engineering Ltd.

Vinagre-Sendino J, Curran T, Crickley S. Preliminary sewage sludge inventory and compilation (**PhD**). Irish Research Council Employment Based Postgraduate Scheme in collaboration with WEW Engineering Ltd.

Zhang L, Grace P. Preliminary studies on sorption isotherms of apples and pear at 25°C (**PhD**). China Scholarship Council (CSC) and University College Dublin (UCD).

Zhao YM, de Alba Ortega M, Sun DW, Tiwari B. Quality evaluation of mackerel fillets after high pressure treatment (**PhD**). China Scholarship Council (CSC) and University College Dublin (UCD).

Appendix 2

Profiles of Postdoctoral Research Scholars only includes: Drs, Alattar; Ktenioudaki; Langreo; Martinez-Gonzalez; O'Connell; Oldfield; Zhao, and Mr White.

Nebras Alattar, BSc,MSc, PhD Physics

Project Title: Chemical Imaging and Chemometrics to Accelerate and Improve Patient Prostate Biopsy Assessment for Cancer.

Project Leader: Associate Prof. Aoife Gowen

Abstract

Currently diagnostic and therapy methods are often limited by insufficient sensitivity, specificity and spatial resolution, depending upon staining processes to illustrate important features of a biopsy. Chemical imaging has potential for the diagnosis and prognosis of cancer based on direct characterisation of the biochemistry of a biopsy sample. The aim of this work is to combine Raman Chemical Imaging with conventional methods (immunohistochemistry) to generate highly detailed chemical images that contain imperceptible biochemical information from the prostate tissue. Raman chemical images are acquired using a Raman microscope with spatial mapping ability to provide a detailed chemical map over the surface of a sample. Three multivariate analysis (MVA) methods; Independent Component Analysis (ICA), Partial Least Squares (PLS) and K-means, are employed here to generate chemical images. Integrating the chemical images with existing digital pathology and patient medical histories have been proposed to generate predictive models of patient outcomes from pre-radical prostatectomy data.

Background, Skills & Qualifications

I obtained a BSc in Physics, in 1997, from Almustansiriyah University-Baghdad and MSc in physics, in the field of optics & lasers, in 2002 from University of Baghdad. I have joined the department of laser and optoelectronics /university of technology-Baghdad as assistant lecturer in 2005. In 2010, I have awarded a scholarship funded from the ministry of higher education-Iraq to obtain PhD degree in UCD. I obtained the PhD from school of physics/UCD in early 2015. My thesis, was centred on the development of a multifunctional microscope which has applications in spanning fluorescence imaging, Raman spectroscopy, fluorescence correlation spectroscopy, time correlated single photon counting, and Raman imaging. Following my PhD, I was awarded a post doc position funded by SFI, focusing on the development of an optical system for investigation and sensing the pathological bacteria. This experience helped me to develop an image analysis modulus, in the field of the digital pathology, in my next post-doctoral fellow role. This modulus would quantify protein expression in tumour/non-tumour areas, was generated by immunohistochemistry methodology. Currently, I am working with associate prof. Aoife Gowen in spectral imaging research group as a post doc funded by HRB.

Selected Recent Publications

Al-attar, Nebras, Rusul M. Al-Shammari, Michele Manzo, Katia Gallo, Brian J. Rodriguez, and James H. Rice. (2018). 'Wide-Field Surface-Enhanced Raman Scattering from Ferroelectrically Defined Au Nanoparticle Microarrays for Optical Sensing': AF2M.5.

Al-Shammari, R. M., M. A. Baghban, ***N. Alattar***, A. A. Gowen, K. Gallo, J. H. Rice, and B. J. Rodriguez. (2018). 'Photo-Induced Enhanced Raman from Lithium Niobate on Insulator Template', ACS Appl Mater Interfaces.

Malallah, Ra'ed, Haoyu Li, Inbarasan Muniraj, Derek Cassidy, ***Nebras Al-Attar***, John J. Healy, and John T. Sheridan. (2018). 'Controlling the trajectories of self-written waveguides in photopolymer', Journal of the Optical Society of America B, 35.

Anastasia Ktenioudaki, BSc, MSc, PhD

Project title: A real-time forecast decision support system for the food supply chain (FreshProof)

Project Leader: Professor Colm P. O'Donnell

Abstract
The project focuses on an innovative systems approach to address existing food supply chain waste and shortcomings in food safety, integrity and traceability. Data on critical environmental conditions in the field and during processing and distribution of fresh fruit and vegetables, will be collected and merged with data on products quality attributes, nutritional value and shelf-life performance. The project is aiming to combine both pre- and postharvest conditions in a single decision support tool, implementing prediction models to determine the remaining shelf-life and nutritional value of a product to consumer level.

Background, Qualifications and Skills
My current research is funded by the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Global Fellowship grant. I am currently hosted at the Food Quality Laboratory, University of South Florida, Tampa, USA. I obtained a PhD in Biosystems Engineering from University College Dublin in 2008, which assessed novel rheological and physical/chemical techniques for wheat quality evaluation.

Since graduating I have worked in multidisciplinary research projects as a research officer and post-doctoral researcher at Teagasc Food research Centre, Ashtown; and I had the opportunity to lead NPD and research projects in my previous role as a senior research and development scientist at Kerry Global Technology and Innovation Centre, Ireland. My research projects have mainly been in the areas of food engineering and food science focusing on the development of new quantitative and qualitative methodologies for assessing product quality, monitoring shelf-life and investigating physicochemical and nutritional properties of food and food molecular structure.

Previous studies include an MSc in Biosystems Engineering from UCD and a BSc in Agriculture from Aristotle University of Thessaloniki, Greece.

Recent Publications
Mc Carthy U., Uysal I., Mercier S., Badia R., **Ktenioudaki A**., O'Donnell C. (2018). Global food security – Issues, challenges and technological solutions. *Trends in Food Science and Technology*, Under Review

O'Shea N, **Ktenioudaki A**, Smyth TP, McLoughlin P, Doran L, Auty, M. A. E., Arendt, E., Gallagher, E., (2015). Physicochemical assessment of two fruit by-products as functional ingredients: Apple and orange pomace. *Journal of Food Engineering,* 153:89-95

Ktenioudaki A, Alvarez-Jubete L, Smyth TJ, Kilcawley K, Rai DK, Gallagher E. (2015). Application of bioprocessing techniques (sourdough fermentation and technological aids) for brewer's spent grain breads. *Food Research International*, 73:107-16

Ktenioudaki A, Alvarez-Jubete L, Gallagher E. (2015). A Review of the Process-Induced Changes in the Phytochemical Content of Cereal Grains: The Breadmaking Process. *Critical Reviews in Food Science and Nutrition,* 55:611-9

Ktenioudaki A, O'Shea N, Gallagher E. (2013). Rheological properties of wheat dough supplemented with functional by-products of food processing: Brewer's spent grain and apple pomace. *Journal of Food Engineering*, 116:362-8

Ana Herrero-Langreo, BSC, M.EngSc, PhD

Project Title: Multi-scale hyperspectral imaging for enhanced understanding and control of food microbiology (HyperMicroMacro)

Project Leader: Assoc. Prof. Aoife Gowen and Assoc. Prof. Amalia Scanell

Abstract

HyperMicroMacro addresses critical gaps in our knowledge of food safety by developing new understanding of the growth and persistence of bacteria, spores and biofilms on surfaces. The overarching aim of this project is to create the knowledge base required to develop a user-friendly hand-held device, capable of detecting and identifying microbes on a range of surfaces. We will address these questions using hyperspectral imaging (HSI) at multiple spatial scales (from microscopic to macroscopic) and spectral modalities (e.g. Raman, IR and Fluorescence) combined with microbial characterisation and high throughput sequencing (HTS). This approach will provide new insights on the persistence of food related microorganisms and their behaviour on foods and other surfaces. The knowledge developed will allow us to develop a prototype rapid detection system to improve safety and security of the food chain. Funding for this research was provided by Science Foundation Ireland (SFI) under the investigators programme Proposal ID 15/IA/2984

Background, Skills & Qualifications

Ana finished her PhD in non-destructive assessment of fruit quality in 2010 in Universidad Politécnica de Madrid (Spain). During her PhD thesis, she combined expert knowledge on fruit maturation physiological processes with applied multivariate analysis to develop, evaluate and select non-destructive sensors for the assessment of fruit and vegetable quality at postharvest (Herrero-Langreo et al., 2012). Throughout this period, she studied physical and chemical properties of fruits and vegetables through their rheological and optical properties and specialised in chemometric data analyses, particularly regarding modelling, classification, spectroscopy and hyperspectral image analysis. Since then, she has worked in between the disciplines of agronomy, food science, and multivariate data analysis in a wide variety of applications, including Fruit and Vegetables Quality Assessment, Precision Agriculture and Plant breeding programs. Some examples of her research are the adaptation of sampling methods to the calibration of spatial models in precision viticulture, (Herrero-Langreo et al., 2018); the assessment and improvement of NIR model robustness for plant breeding purposes; and the development of multispectral indexes for spectral imaging (Mishra et al., 2015). Her current research at UCD focuses on the application of hyperspectral imaging for the investigation of microbial growth in food matrices, exploration of different spectral modalities at different scales and development of adapted chemometric approaches for developing new understanding of the growth and persistence of bacteria, spores and biofilms on surfaces.

Selected Recent Publications

Herrero-Langreo A., Fernández-Ahumada E., Roger J.M., Palagós B., Lleó L. (2012). Combination of Optical and Non-destructive Mechanical Techniques for the Measurement of Maturity in Peach, *Journal of Food Engineering*, 108 (1), 150-157, 10.1016/j.jfoodeng.2011.07.004.

Mishra P., **Herrero-Langreo A**., Barreiro P., Roger J.M., Diezma B., Gorretta N., Lleó L. (2015). Hyperspectral to Multispectral Imaging for Detection of Tree Nuts and Peanut Traces in Wheat Flour. Journal of Near Infrared Spectroscopy. *Journal of Spectral Imaging* (4).10.1255/jsi.2015.a2

Herrero-Langreo A., Tisseyre B., Roger J.M., Scholasch T., Payen S., (2018) Test of Sampling Methods to Optimize the Calibration of Vine Water Status Spatial Models. **Precision Agriculture**. 19 (2), 365-378.

José Ángel Martínez-González, BSc, MSc, PhD

Project Title: BIOWATER PROJECT: Theoretical and experimental approaches to unravel the water structure at biomaterial interfaces

Project Leader: Dr. Aoife Gowen

Abstract
This project evaluates the use of Molecular Dynamics (MD) in combination with hyperspectral imaging techniques to provide a deeper understanding of the molecular structure of water at biomaterial interfaces and how this structure is conditioned according to the properties of the biomaterial. MD is a theoretical approach for studying atoms and molecules along a fixed period of time giving a view of the dynamical evolution of the system. MD simulations have many applications, e.g. refine three-dimensional experimental structures from X-ray or NMR (such as proteins or macromolecules) or to understand the growth of thin films. Combining this technique with IR and Raman hyperspectral imaging techniques allow us to obtain a better understanding of the processes that occur in the interfacial zones from a macroscopic and atomic point of view. Additionally, non-equilibrium MD simulations help us to elucidate the key role that water adopts in protein adsorption from the atomic level perspective.

Background, Skills & Qualifications
I completed my PhD in Chemistry at University of La Rioja in 2013, with a study of the reaction mechanism and kinetics of hepatitis C virus NS3/NS4A protease applying several theoretical approaches to elucidate the enzymatic reaction mechanism. Until January 2015, I was working in the soft matter field, focusing on the amorphization of silica family derivatives and electronic characterization of these materials at the University Autónoma de Barcelona. From September 2016 to June 2018, I have been working in the UCD where I have been simulating the interface between silicon based materials with water to characterize the theoretical infrared spectrum of this interface. Recently, I obtained a Marie-Skłodowska Curie Fellow under Rutherford International Fellowship Programme to continue researching at Science and Technology Facilities Council in United Kingdom.

Recent publications
Martínez-González, J.A.; Navarro-Ruiz, J. & Rimola, A. (2018). *Multiscale Computational Simulation of Amorphous Silicates' Structural, Dielectric, and Vibrational Spectroscopic Properties.* Minerals, 8:353.

Mukherjee, S; **Martínez-Gonzalez, J.A**.; Dowling, D.P. & Gowen, A.A. (2018). *Predictive modelling of water contact angle of surfaces using Attenuated Total Reflection – Fourier Transform Infrared (ATR-FTIR) chemical imaging and Partial Least Squares Regression (PLSR)* Analyst, 143:3729-3740.

Martínez-Gonzalez, J.A.; English, NJ & Gowen, A.A. (2017). *Understanding the interface between silicon-based materials and water: molecular-dynamics exploration of infrared spectra.* AIP Advances, 2017,7:115105

Mukherjee, S; Martínez-Gonzalez, J.A.; Stallard, C.P.; Dowling, D.P. & Gowen, A.A. (2017). *Can ATR-FTIR be Used To Understand The Interaction Between Polymers And Water? A Hyperspectral Imaging Study.* Journal of Spectral Imaging. DOI: 10.1255/jsi.2017.a3

Martínez-Gonzalez, J.A.; González, M.; Masgrau, L. & Martinez, R. (2015). *Theoretical Study of the Free Energy Surface and Kinetics of the Hepatitis C Virus NS3/NS4A Serine Protease Reaction with the NS5A/ 5B Substrate. Does the Generally Accepted Tetrahedral Intermediate Really Exist?* ACS Catalysis, 5:246-255.

Jerome O'Connell BSc, MSc, PhD

Project Title: GeoHub: Radiometric normalisation of image data for vehicle or UAV mounted sensors

Project Leader: Prof. Nick Holden

Abstract
The global market for remote sensing is projected to grow from $8.1B in 2014 to $12.1B by 2019. The move towards integration of remote sensing and other big data sources into day to day decision making in industries like precision agriculture has been clearly demonstrated by large multinational investment. However, several roadblocks (e.g. data quality and consistency and data integration/compatibility) have been identified by industry and academics which is prohibiting the widespread uptake of such data in sectors like agriculture. GeoHub will create a dedicated software solution for maintaining data quality and compatibility for such platforms, thereby facilitating the widespread integration of such data into industries like precision agriculture and natural resources.

Background, Qualifications and Skills
My main research interest lies in the commercial and scientific application of remote sensing in agriculture and natural resources. In particular, the development of image processing tools and software around radiometric correction, image classification, image enhancement and data transfer. I graduated in December 2007 with a Masters in Applied Science in GIS and Remote Sensing in Environmental Management at University College Cork. In addition, I was also awarded a Masters in Forestry from the University of Wales, Bangor in 2005. I completed my PhD in University College Dublin in 2012. The main objective of this research was to create a monitoring protocol for the detection of disturbance in Irish peatlands. In November 2016, I completed a 4 year post doctorate in the University of Leeds on habitat mapping in agricultural landscapes. I am also involved in other collaborations, including work with New York University on conservation agriculture in Malawi and the EU-BON pan-European biodiversity observation network.

Recent Publications
O Connell, J., Bradter, U. and Benton, T. G. 2015. Wide-area mapping of small-scale features in agricultural landscapes using airborne remote sensing. *ISPRS Journal of Photogrammetry and Remote Sensing*, 109, 165-177.

O Connell, J., Connolly, J. and Holden, N. 2014. A monitoring protocol for vegetation change on Irish peatland and heath. *International Journal of Applied Earth Observation and Geoinformation*, 31, 130-142.

O Connell, J., Bradter, U. and Benton, T. G. 2013. Using high resolution CIR imagery in the classification of non-cropped areas in agricultural landscapes in the UK. *SPIE Remote Sensing.* Dresden, Germany, International Society for Optics and Photonics.

O Connell, J., *et al.*, 2013. Radiometric normalization for change detection in peatlands: a modified temporal invariant cluster approach. *International Journal of Remote Sensing*, 34, 2905-2924.

Tom Oldfield, BSc, MSc, PhD.

Project Title: AgroCycle

Project Leader: Professor Shane Ward, Dr Tom Curran

Abstract

Continuing population and consumption growth are driving global food demand, with agricultural activity expanding to keep pace. The modern agricultural system is wasteful, with Europe generating some 700 million tonnes of agrifood waste each year along the entire agrifood production chain. The AgroCycle project will further develop, demonstrate and validate novel processes, practices and products for the sustainable use of agricultural wastes in applications such as fertilisers, biopolymers and novel chemicals as well as developing technology and policy guidelines for the bioeconomy. The project's holistic approach will also include significant life cycle assessment work to evaluate the environmental performance that is crucial in determining the suitability and sustainability of potential value chains.

Background, Skills & Qualification

My PhD thesis, regarding the analysis of organic waste was completed in 2016 under the supervision of Professor Nicholas Holden at UCD. This focused on how life cycle assessment is used to analyse waste management and waste valorisation pathways, and a number of case studies were undertaken for Ireland, Europe and California. I obtained an MSc in Sustinable Energy and Green Technology from UCD in 2012 and a BSc in International Disaster and Engineering Management from Coventry University in 2008.

Recent publications

Toop, T., Ward, S., **Oldfield, T.L**., Hull, M., Kirby, M.E., Theodorou, M.K. (2017)**.** AgroCycle – developing a circular economy in agriculture. Energ. Procedia.

Oldfield *et al.* (2017). The implications of stakeholder perspective for LCA of wasted food and green waste. *J. of Clean. Prod.*

Oldfield, *et al*. (2017). A life cycle assessment of biosolarization as a valorization pathway for tomato pomace utilization in California. *J. of Clean. Prod*. 141, 146-156.

Ward, S., Holden, N.M., White, E., **Oldfield, T.L. (**2017)**.** Agriculture. Waste to resource. Report for UK Chief Scientific Officer.

Ming Zhao, BSc, MEnSc., PhD

Project Title: Process analytical technology (PAT) for on-line quality control of dairy products

Project Leader: Prof. Colm O'Donnell

Abstract

PAT encompasses analytical measurements and understanding of chemical, physical and microbiological parameters governing industrial processing. With regard to the dairy industry, critical PAT considerations include quality and authenticity for at-line, inline and on-line monitoring purposes. This project evaluates the potential of spectroscopic techniques combined with chemometric analysis for the prediction of main ingredients and contaminations of infant formula and milk products.

Background, Skills & Qualifications

My PhD thesis, concerning development of PAT tools using a range of spectral and chemometric approaches for advanced process control and adulteration detection in selected beef and dairy products, was completed in 2016 under the supervision of Prof. Colm O'Donnell and Prof. Gerard Downey in UCD. This work involved: spectroscopic techniques (NIR, MIR, Raman, microwave and hyperspectral imaging) with chemometric approaches for in-line, on-line or at-line use in the meat and dairy industry. I obtained an MEnSc in Food and Biosystems Engineering from UCD in 2012 and a BSc in Nutritional Science from UCC in 2010.

Recent publications

Yuanyuan Pu, **Ming Zhao**, Colm P. O'Donnell, Da-Wen Sun (2018). Nondestructive quality evaluation of banana slices during microwave vacuum drying using spectral and imaging techniques. *Drying Technology*. Published online: 08 Feb 2018. https://doi.org/10.1080/07373937.2017.1415929

Ming Zhao, Yingqun Nian, Paul Allen, Gerard Downey, Joseph P. Kerry, Colm P. O'Donnell (2018). Application of Raman spectroscopy and chemometric techniques to assess sensory characteristics of young dairy bull beef. *Food Research International*, 107, 27-40.

Yingqun Nian, **Ming Zhao**, Colm P. O'Donnell, Gerard Downey, Joseph P. Kerry, Paul Allen (2017). Assessment of physico-chemical traits related to eating quality of young dairy bull beef at different ageing times using Raman spectroscopy and chemometrics. *Food Research International*, 99, 778-789.

Ming Zhao, Carlos Esquerre, Gerard Downey, Colm P. O'Donnell. (2016). Process analytical technologies for fat and moisture determination in ground beef - a comparison of guided microwave spectroscopy and near infrared hyperspectral imaging. *Food Control*, 73, 1082-1094.

Ming Zhao, Gerard Downey, Colm P. O'Donnell. (2016). Exploration of microwave dielectric and near infrared spectroscopy with multivariate data analysis for fat content determination in ground beef. *Food Control*, 68, 260-270.

Eoin White, BE, M.Sc.

Project Title: AgroCycle

Project Leader: Dr. Tom Curran, Prof. Shane Ward

Abstract

The AgroCycle project addresses the application of the 'circular economy' across the agri-food sector. The 'circular economy' aims to reduce waste while also making best use of the 'wastes' produced – the so called 'valorisation' of waste. The project will develop, demonstrate and validate novel processes, practices and products for the sustainable use of agricultural wastes in applications such as fertilisers, biopolymers and novel chemicals as well as developing technology and policy guidelines for the bioeconomy. Specific tasks that I have undertaken thus far have been mapping under-valorised waste streams in the agricultural production and supply chain across Europe and helping to develop detailed databases to store and present this data. I conducted a holistic analysis on the impact of removing AWCB on agricultural systems, and logistics issues. Sustainable removal ratios were calculated for common agricultural commodities and the main AWCB classified into categories based on whether they can be avoided and on whether it is technically feasible to be collected. These works have been published through AgroCycle deliverables and presented at the 2018 European Open Science Forum

Background, Skills & Qualifications

I am a life cycle assessment specialist with particular experience in the areas of industrial ecology and circular economy. I have worked with organization to help quantify and communicate their environmental performance in both consulting and research roles. I obtained a M.Sc. in Industrial Ecology from Leiden University in 2014 with my thesis being completed at Shell Global Solutions in Amsterdam on the topic of developing life cycle energy metrics to evaluate energy technologies. I hold a BE in Biosystems Engineering from UCD. I'm currently a part-time contract researcher with the AgroCycle project where I assist with technical project management and research in addition to academic and policy dissemination.

Selected Recent Publications

Ward, S. M., Holden, N. M., **White, E. P**., Oldfield, T. L. (2017) From Waste to Resource Productivity, Chapter 6 Agriculture. Annual Report of Government Chief Scientific Adviser. Government office for Science

Oldfield, T. L., **White, E**.**P**, Holden N. M. (2016) An environmental analysis of options for utilising wasted food and food residue. Journal of Environmental Management 183: 826-835