

IASIM 2022

Conference on spectral imaging
3–6 July, Esbjerg, Denmark

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Welcome to IASIM-2022

On behalf of the International Association for Spectral Imaging (IASIM), we have a pleasure to welcome you at IASIM-2022 — the eighth international conference in spectral imaging.

The biannual IASIM conference is intended to provide a unified, open, cross-disciplinary and interactive forum for the exchange of information and ideas within the general spectral imaging community, regardless of the spectral or spatial range.

Scientific sessions will include keynote presentations by invited speakers, contributed presentations, panel discussions from members of the imaging community, posters and exhibitors, promoting cross-talks and new ideas.

Presenters of mature works will be encouraged to submit their manuscripts for publication in the special issue of *Journal of Spectral Imaging*, subject to the normal peer review process.

We hope you will enjoy the conference!

IASIM scientific committee

- Aoife Gowen, *University College Dublin*
- Ana Maria De Juan Capdevila, *University of Barcelona*
- Federico Marini, *University of Rome “La Sapienza”*
- Paolo Oliveri, *University of Genova*
- Cyril Ruckebusch, *University of Lille*
- Ludovic Duponchel, *University of Lille*
- Bosoon Park, *University of Athens, Georgia, USA*
- Neal Gallagher, *Eigenvector Research*
- Sergey Kucheryavskiy, *Aalborg University*
- Jose Manuel Amigo Rubio, *University of the Basque Country*

Conference programme

All scientific activities will take place in the **Musikhuset Esbjerg** (*Havnegade 18*). Just take the main entrance and then stairs down (follow the indication you will find there). The oral sessions will be located in the conference hall while the poster session, exhibition and coffee-breaks in the lounge area outside the hall.

Please have you conference badge on during all sessions and events. It serves also as a ticket to the excursion and the conference dinner.

Sunday, 3/07

13:00–14:00	Registration	
14:00–15:20	Hands-on LED spectral imaging By Videometer Exhibition area	Using HYPER-Tools for analysis of hyperspectral images By Jose Manuel Amigo Rubio Conference hall
15:40–17:00	Live demonstration of how to build a HSI real-time application By Hypspec/NEO/Prediktera Exhibition area	The workshop will be from 14:00 to 17:00 with breaks in between.
17:00–19:00	Welcome reception	

Monday, 4/07

8:00–9:00 Registration

9:00–9:10 Conference opening

Session 1. Chair *Anna de Juan*

9:10–9:50 **L01. Medical Hyperspectral Imaging**

Baowei Fei : University of Texas at Dallas

9:50–10:10 **T01. Combining Raman hyperspectral imaging with mass spectrometry imaging to differentiate involved from non-involved skin in discoid lupus erythematosus (dle)**

Michel Karin Nieuwoudt : University of Auckland

10:10–10:30 **T02. Non-destructive age estimation of biological fluid stains by near-infrared hyperspectral imaging and multivariate regression**

Paolo Oliveri : University of Genova

10:30–11:00 Coffee break

11:00–11:40 **T03. NIR hyperspectral imaging: a means of capturing meat fraud**

Paul James Williams : Stellenbosch University

11:20–11:20 **T04. Monitoring grape berry maturity by hyperspectral imaging: potential of robust methods for sugar content prediction**

Maxime Ryckewaert : INRAE

11:40–12:00 **T05. Hyperspectral imaging for non-invasive fish fraud detection**

Mariá-José Sáiz-Abajo : National Centre for Food Technology and Safety

12:00–12:20 **T06. Unsupervised anomaly detection in hyperspectral images of fruit by adapting a vector quantized variational autoencoder**

Remi Van Belleghem : KU Leuven

12:20–13:00 Lunch

Session 2: Chair *Ludovic Duponchel*

13:00–13:40 **L02. Hyperspectral imagery: applications in remote sensing**

Mauro Dalla Mura : Grenoble Institute of Technology

13:40–14:00 **T07. Hyperspectral-LIDAR fusion applied for multitemporal analysis of urban areas**

Agnieszka Kinga Kuras : Norwegian University of Life Sciences

14:00–14:20 **T08. Hyperspectral imaging in nuclear forensics investigation**

Lorenzo Fongaro : European Commission

14:20–14:50 Coffee-break

- 14:50–15:10 **T09. Spatial and spectral limits of detection of near infrared hyperspectral imaging of microplastics in sand**
Reaha Goyetche : University of the Basque Country
- 15:10–15:30 **T10. Using hyperspectral cameras to detect corrosion products in epoxy coatings for offshore wind turbines**
Thomas De Kerf : University of Antwerpen
- 15:30–15:50 **T11. Characterizing Ni-P metallic coatings using hyperspectral imaging in short-wave infrared**
Zohreh Zahiri : University of Antwerpen
- 15:50–16:10 **T12. Plastic classification via in-line hyperspectral camera analysis and unsupervised machine learning**
Mogens Hinge : Aarhus University
- 16:10–18:00 **Poster session and exhibition**
with tasting of local beers (sponsored by Newtec Engineering)

Tuesday, 5/07

9:00–9:10 Welcome and day overview

Session 3: Chair *Federico Marini*

- 9:10–9:50 **L03. Reflectance Imaging Spectroscopy for artworks, cultural and historical assets**
Costanza Cucci : Institute of Applied Physics "N. Carrara" CNR-IFAC
- 9:50–10:10 **T13. HSI-NIR for the quantification of collagen in bones: how chemical mapping can help in preserving archeological finds**
Cristina Malegori : University of Genova
- 10:10–10:30 **T14. Comparison of reflectance FTIR, VNIR and SWIR spectral imaging for the discrimination and identification of bacterial suspensions dried on stainless steel**
Aoife Ann Gowen : University College Dublin
- 10:30–11:00 Coffee break
- 11:00–11:20 **T15. Detection of *cronobacter sakasakii* biofilms on aluminium coupons through ultrafast FTIR spectral imaging**
Ana Herrero-Langreo : University College Dublin
- 11:20–11:40 **T16. In-line identification of PB-based additives in fishing ropes and nets for recycling with hyperspectral imaging and machine learning**
Georgiana Amariei : Aarhus University

- 11:40–12:00 **T17. Characterization of microplastics in mussels using near infrared hyperspectral imaging**
Alisa Rudnitskaya : University of Aveiro
- 12:00–12:20 **T18. Parsketch-PLSDA, a method to handle large amounts of data generated by hyperspectral imaging: application to sunflower genotype discrimination**
Daphne Heran : INRAE
- 12:20–13:00 Lunch

Session 4: Chair *Jose Manuel Amigo Rubio*

- 13:00–13:20 **T19. Correcting time-induced measurement effects in NIRS model: application to the early detection of “early blight”**
Florent Abdelghafour : INRAE
- 13:20–13:40 **T20. Characterization of N-doped diamonds after electron beam irradiation by infrared spectral imaging**
Tom Scherzer : Leibniz Institute of Surface Engineering
- 13:40–14:00 **T21. Spectral imaging as a transformer of the food-ag industry**
Jens Michael Carstensen : Videometer A/S
- 14:00–14:20 **T22. One-step calibration of industrial hyperspectral cameras**
Martin Lahn Henriksen : Aarhus University

14:20–14:50 Coffee-break

14:50–16:00 **Poster session and exhibition**

16:00–18:00 **Bus tour and excursion to Ribe — the oldest town in Scandinavia**
bus will wait just outside the main entrance of Musikhuset

18:00–19:00 **Free time**

19:00–22:00 **Conference dinner at Restaurant Flammen**
Exnersgade 20, Esbjerg

Wednesday, 6/07

9:00–9:10 Welcome and day overview

Session 5: Chair *Aoife Gowen*

- 9:10–9:50 **L04. Raman Imaging: fundamentals, modern applications and future perspectives**
Marco Veneranda : University of Valladolid
- 9:50–10:10 **T23. Searching for exotic pixels in large hyperspectral imaging data sets**
Ludovic Duponchel : University of Lille

10:10–10:30 **T24. Automatic parasite detection in fish using hyperspectral imaging**
Andreas Vidman : Prediktera AB

10:30–11:00 Coffee break

11:00–11:20 **T25. Quantitative analysis of hyperspectral images: some new insights**
Anna de Juan : University of Barcelona

11:20–11:40 **T26. Recent advances in high-resolution snapshot computed tomography imaging spectrometer**
Mads Svanborg Peters : University of Southern Denmark

11:40–12:00 **T27. Comparison of strategies for pixel selection for single- and multi-block image modeling**
Federico Marini : University of Rome "La Sapienza"

12:00–12:20 **T28. Sparse non-negative matrix factorization of hyperspectral images down to essential pixels**
Mahdiyeh Ghaffari : Radboud University

12:20–13:00 Lunch

Session 6: Chair *Paolo Oliveri*

13:00–13:20 **T29. Tomographic reconstruction of hyperspectral images - a hybrid approach using CNNs and the EM algorithm**
Mads Juul Ahlebaek : University of Southern Denmark

13:20–13:40 **T30. Join data polytope analysis of multimodal hyperspectral images**
Nematollah Omidikia : Radboud University

13:40–14:00 **T31. Multi-spectral refuse segmentation for refuse sorting systems**
Franz Thaler : Graz University of Technology

14:00–14:20 **T32. Mathematical nuances of Generalized Least Squares**
Jose Manuel Amigo Rubio : University of the Basque Country

14:20–14:50 Conference closing and farewell

L01. MEDICAL HYPERSPECTRAL IMAGING

Baowei Fei

University of Texas at Dallas, Department of Bioengineering, Richardson, Texas, USA

University of Texas Southwestern Medical Center, Department of Radiology, Dallas, Texas, USA

Hyperspectral imaging (HSI) is an emerging imaging modality for medical applications, especially in disease detection, diagnosis, and treatment [1]. HSI acquires a three-dimensional dataset called hypercube, with two spatial dimensions and one spectral dimension. Spatially resolved spectral imaging obtained by HSI provides physiopathological information about tissue condition and composition, which can be used to detect various diseases. Particular applications of hyperspectral imaging include cancer detection & diagnosis [2], image-guided surgery [3], and computational & digital pathology [4].

In this talk, various hyperspectral imaging technologies and their medical and biological applications will be presented and discussed. One particular application is on the detection of head and neck squamous cell carcinoma (SCC). Machine learning and quantification methods are developed and applied to the HSI data. HSI for image-guided surgery will be demonstrated. Promising results from both preclinical and clinical studies will be included in this talk. It has been demonstrated that label-free, reflectance-based HSI can accurately detect the cancer margin in tissue specimens. This non-ionizing optical imaging modality could aid surgeons and reduce inadequate surgical margins during SCC resections. Future directions and potential challenges of medical hyperspectral imaging will be discussed.

References

1. G. Lu, B. Fei. Medical hyperspectral imaging: a review. *J Biomed Opt.* 2014, 19(1) 10901.
2. M. Halicek, H. Fabelo, S. Ortega, G.M. Callico, B. Fei. In-vivo and ex-vivo tissue analysis through hyperspectral imaging techniques: revealing the invisible features of cancer. *Cancers (Basel)*. 2019, 11(6):756.
3. B. Fei, G. Lu, X. Wang, H. Zhang, J.V. Little, M.R. Patel, C.C. Griffith, M.W. El-Diery, A.Y. Chen. Label-free reflectance hyperspectral imaging for tumor margin assessment: a pilot study on surgical specimens of cancer patients. *J Biomed Opt.* 2017 22(8):1-7.
4. S. Ortega, M. Halicek, H. Fabelo, G.M. Callico, B. Fei. Hyperspectral and multispectral imaging in digital and computational pathology: a systematic review, *Biomed Opt Express*. 2020, 11(6):3195-3233.

L02. HYPERSPECTRAL IMAGERY: APPLICATIONS IN REMOTE SENSING

Mauro Dalla Mura

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Institut Universitaire de France (IUF), France

Hyperspectral imagery is a rising technology in remote sensing, addressing tasks from the characterization of the natural environment [1] (e.g., vegetation, coastal areas and cryosphere) to the monitoring of anthropic activities [2] (e.g., in urban areas, agriculture or atmosphere).

This talk will be devoted to give an overview on the application of hyperspectral imagery in remote sensing by presenting the main advantages of this technology, the challenges and some examples of how to address them.

References

1. T. Bajjouk, F. de Boissieu, J. Chanussot, S. Dout, M. Dumont, J.-B. Féret, T. Masson, A. Minghelli, P. Mouquet, F. Schmidt, M. Dalla Mura, “Chapter 3.1 - Applications in remote sensing—natural landscapes”, *Hyperspectral Imaging*, Editor: José Manuel Amigo, Elsevier, Volume 32, 2019, Pages 371-410, <https://doi.org/10.1016/B978-0-444-63977-6.00016-X>.
2. J. Aval, X. Briottet, S. Fabre, P.-Y. Foucher, V. Carrère, R. Marion, K. Uto, C. Weber, M. Dalla Mura, “Chapter 3.2 - Applications in remote sensing—anthropogenic activities”, *Hyperspectral Imaging*, Editor: José Manuel Amigo, Elsevier, Volume 32, 2019, Pages 411-452, <https://doi.org/10.1016/B978-0-444-63977-6.00017-1>.

L03. REFLECTANCE IMAGING SPECTROSCOPY FOR ARTWORKS, CULTURAL AND HISTORICAL ASSETS

Costanza Cucci

Institute of Applied Physics “N. Carrara” (IFAC), National Research Council, Florence, Italy

Over the last decades Imaging Spectroscopy (IS) has gained increasing importance in the field of Cultural Heritage, taking shape today as a novel, well-structured research area. Among the IS techniques, the Vis-NIR and SWIR reflectance HyperSpectral Imaging (HSI) is today acknowledged as one of the most comprehensive methodologies for non-invasive and extensive investigation of polychrome surfaces and their underneath layers [1,2].



Fig. 1. Reflectance Hyperspectral Imaging IFAC-CNR Scanner. Measurements on a Renaissance painting (1450 ca) from the Florentine School of Beato Angelico. Soprintendenza Labs, Uffizi Gallery (Firenze).

Initially reserved to the study of paintings, after an extraordinary technological maturation, in latest years reflectance HSI has been extended to novel applications, from indoor museum objects (paintings, manuscripts, but also coffins and historical objects, etc.) up to open environments (wall paintings, ceilings, archaeological sites, etc.) [3]. HSI data-cubes include high-resolution spatial and spectral information, which is usable not only for the identification and mapping of pigments and artists' materials, and for the inspection of hidden details in painted surfaces (underdrawings, *pentimenti*, signatures, etc.), but also for retrieving ancient texts, faded inscriptions, or assessing the conservation status and degradation of surfaces. Thus, reflectance HSI has become a pivotal technique in the multi-modal analytical protocols adopted in major museums [4]. Also, the technique is regarded with high interest for its potentialities in the field of Virtual Museums. The growing use of HSI in museum contexts has also stimulated research on topics related to HSI data-handling, processing and exploitation, as well as data-fusion with other techniques. A thriving research direction is today looking for algorithms specifically tailored for the HSI-data-cubes acquired on paintings. Currently, this research area is focusing on solutions borrowed from the Artificial Intelligence (AI) methods, aimed at the automatic data-processing of big-size HSI data-sets acquired on paintings [5].

The lecture will be an introduction to the ever-increasing use of reflectance HSI in the field of Cultural Heritage. The specific issues related to the implementation of HSI technique for investigating artworks will be reviewed, going through examples of case-studies selected from prestigious museums and cultural contexts (Uffizi Gallery, Pompeii archeological site, Museu Picasso, etc.). The lecture will aim at keeping an open view on main technological challenges, unsolved questions and future perspectives.

References

1. C. Cucci, J. K. Delaney, M. Picollo. Reflectance hyperspectral imaging for investigation of works of art: old master paintings and illuminated manuscripts. *Accounts of chemical research*. 49.10 (2016) 2070-2079.
2. Cucci, C., Casini, A. (2020). Hyperspectral imaging for artworks investigation. In: J. M. Amigo (Ed.), *Data Handling in Science and Technology* (Vol. 32, pp. 583-604). Elsevier.
3. C. Cucci, M. Picollo, L. Chiarantini et al. Remote-sensing hyperspectral imaging for applications in archaeological areas: Non-invasive investigations on wall paintings and on mural inscriptions in the Pompeii site. *Microchemical Journal*. 158 (2020) 105082.
4. F. Albertin, C. Ruberto, C. Cucci et al. "Ecce Homo" by Antonello da Messina, from non-invasive investigations to data fusion and dissemination. *Scientific Reports*. 11 (2021) 15868.
5. C. Cucci, A. Barucci, L. Stefani, et al. . Reflectance hyperspectral data processing on a set of Picasso paintings: which algorithm provides what? A comparative analysis of multivariate, statistical and artificial intelligence methods. *Proc. SPIE Optics for Arts, Architecture, and Archaeology VIII*. 11784 (2021) 1178404.

L03. RAMAN IMAGING: FROM TERRESTRIAL APPLICATIONS TO PLANETARY EXPLORATION MISSIONS

Marco Veneranda

Universidad de Valladolid (UVA), Department of Condensed Matter Physics, Crystallography and Mineralogy, Valladolid, Spain

Raman imaging is a non-destructive chemical analysis that investigates the spatial distribution of the Raman-active chemical components constituting the designated sample. In this work, strengths and tradeoff of this analytical technique are described by presenting representative examples from different field of research, including medicine, geology,

cultural heritage, and forensic. Furthermore, the most common strategies for spectra pre-processing are detailed, these being of critical importance to optimize the scientific outcome of Raman imaging.

Beyond terrestrial applications, the novel application of Raman imaging in space exploration missions is also introduced. As such, the capabilities of the Sherloc instrument¹ onboard the NASA/Mars 2020 Perseverance rover operating at Jezero Crater (Mars) are presented. As confirmed by the laboratory analysis of terrestrial analogues of Martian geological units² (see Fig. 1), the RLS system onboard the ESA/ExoMars Rosalind Franklin rover could be optimized to perform Raman imaging.

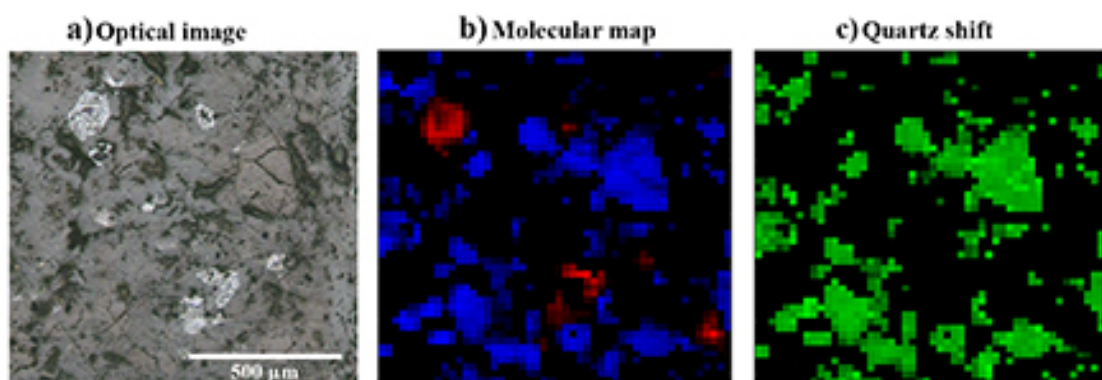


Fig. 1. Raman analysis of a Martian analogue, obtained by the RLS ExoMars Simulator³. a) optical image of the selected area, b) Raman image displaying quartz (blue) and anatase (red) distribution, and c) Raman image displaying the degree of quartz shocking (from M. Veneranda et al. 2019²).

References

1. M. Caffrey et al., IEEE Aerospace Conference. (2020) 1-8.
2. M. Veneranda et al., Astrobiology. 20 (2020) 349-363.
3. Lopez-Reyes, G. et al., J Raman Spectrosc. 53 (2022), 382-395.

T01. COMBINING RAMAN HYPERSPECTRAL IMAGING WITH MASS SPECTROMETRY IMAGING TO DIFFERENTIATE INVOLVED FROM NON-INVOLVED SKIN IN DISCOID LUPUS ERYTHEMATOSUS (DLE)

Michel Nieuwoudt¹⁻⁴, **Hannah Holtkamp**¹⁻³, **Claude Aguergaray**^{1,2,4}, **Satya Amirapu**⁶, **Angus Grey**⁷, **Cather Simpson**¹⁻⁵ and **Paul Jarrett**⁸

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²School of Chemical Sciences, The University of Auckland, New Zealand

³The Dodd Walls Centre for Photonic and Quantum Technologies, New Zealand

⁴The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

⁵Department of Physics, The University of Auckland, New Zealand

⁶Department of Anatomy, The University of Auckland, New Zealand

⁷Department of Physiology, The University of Auckland, New Zealand

⁸Department of Dermatology, Middlemore Hospital, Auckland, New Zealand

⁹Department of Medicine, The University of Auckland, New Zealand Text of the abstract.

DLE is the most common form of cutaneous lupus and causes permanent scarring, scarring alopecia, hyper- or hypo-pigmentary change which is distressing for patients with skin of colour [1]. In this study we combined matrix associated laser desorption ionisation (MALDI) imaging with Raman hyperspectral imaging to differentiate biomarkers in active DLE and clinically normal perilesional skin from the same patient. PCA in HyperTools™ was used to explore and extract the biomolecular information. We found that DLE has a unique epidermal lipid profile with a higher proportion of aromatic acids and specific structural proteins.

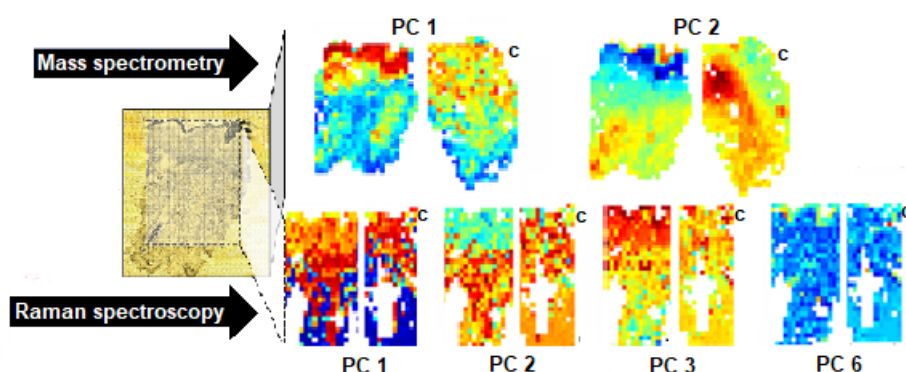


Fig. 1. PCA score images from MALDI and Raman and hyperspectral data of skin sections with active DLE and control section comparison (c)

References

1. Jarrett P, Thornley S, Scragg R. Ethnic differences in the epidemiology of cutaneous lupus erythematosus in New Zealand. *Lupus*. 2016;25(13):1497-502.

T02. NON-DESTRUCTIVE AGE ESTIMATION OF BIOLOGICAL FLUID STAINS BY NEAR-INFRARED HYPERSPECTRAL IMAGING AND MULTIVARIATE REGRESSION

Paolo Oliveri¹, Cristina Malegori¹, Cristina Manis², Eugenio Alladio^{2,3}, Marco Vincenti^{2,3}, Paolo Garofano³, Filippo Barni⁴, Andrea Berti⁴

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³Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Orbassano, Italy

⁴Reparto Carabinieri Investigazioni Scientifiche, Sezione di Biologia, Roma, Italy

From a criminalistic point of view, the accurate dating of biological traces found at the crime scene, together with its compatibility with the estimated crime perpetration timeframe, enables to limit the number of suspects by assessing their alibis and clarifying the sequence of events. The present study delineates the possibility of dating biological fluids such as semen and urine, as well as blood traces, by using a non-destructive analytical strategy based on hyperspectral imaging in the near infrared region (HSI-NIR), coupled with multivariate regression.

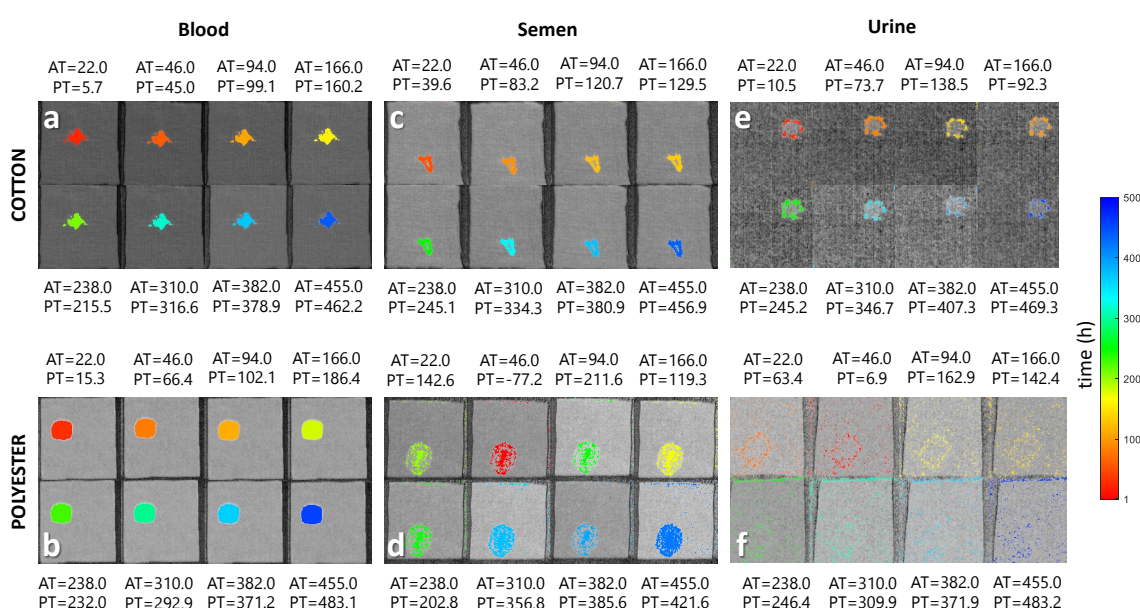


Fig. 1. Color maps related to the different fluids on the two supports. AT = actual time (hours); PT = predicted time (hours) obtained by application of PLS regression.

Investigated aspects of the present study include not only the progressive degradation of the biological trace itself, but also the effects of its interactions with the support on which it is absorbed, in particular the hydrophilic vs. hydrophobic character of fabric tissues. Results are critically discussed, highlighting potential and limitations of the proposed approach for a practical implementation.

T03. NIR HYPERSPECTRAL IMAGING: A MEANS OF CAPTURING MEAT FRAUD

Paul J Williams¹, Kiah Edwards¹, Marena Manley¹, Louwrens C Hoffman^{1,2}

¹Stellenbosch University, Department of Food Science, Stellenbosch, South Africa

²The University of Queensland, Center for Nutrition and Food Science, Queensland, Australia

To protect the consumer, the South African government proposed draft regulations stipulating how much meat must be in their products to be called 'beef patties'. These specify that patties will be divided into four categories: premium 'ground patty' (99.6% meat); regular 'burger patty' (70%+ meat); 'value-burger/patty' (55% meat with $\leq 30\%$ fat) and the 'econo-burger'/'budget' (35% meat with $\leq 30\%$ fat). The 'value-burger' and 'econo-burger' may also contain vegetable protein, mechanically recovered meat and edible offal. Determination of meat content of burger patties is therefore integral.

These draft regulations aim to combat processed meat fraud, however current authentication techniques are destructive, time-consuming and require complex laboratory procedures performed by skilled personnel. Research suggests that an automated spectral imaging camera could perform this process more accurately and with higher through-put [1]. This study aims to provide a rapid and accurate spectral imaging solution for the authentication of processed raw beef patties.

A total of 800 beef patties (200 patties per category) were made and analysed to assess the potential of this technique to distinguish between the four patty categories as well as authenticate the individual patties within each category. Hyperspectral images were acquired with a HySpex SWIR-384 imaging system, in the range of 952 – 2517 nm, after which the data was pre-processed and modelled with various chemometric and machine learning algorithms.

It was possible to distinguish between the four patty categories with accuracies $>97\%$. It was also possible to authenticate the individual patties with accuracies ranging from 90 – 100%. The results showed that NIR HSI combined with multivariate data and image analysis offers

an accurate and reliable technique for the rapid identification and authentication of processed beef patties. Furthermore, this study has the potential of providing an alternative technique to the current manual, destructive and time-consuming methods, thus contributing to the authenticity and fair-trade of processed meat products locally and internationally.

References

1. K. Edwards, M. Manley, L.C. Hoffman, P.J. Williams, Non-Destructive Spectroscopic and Imaging Techniques for the Detection of Processed Meat Fraud, *Foods*. 10 (2021) 448. <https://doi.org/10.3390/foods10020448>.

T04. MONITORING GRAPE BERRY MATURITY BY HYPERSPECTRAL IMAGING: POTENTIAL OF ROBUST METHODS FOR SUGAR CONTENT PREDICTION

*Ryad Bendoula¹, Aldrig Courand¹, Maxime Metz¹, Daphné Héran¹, Carole Feilhes², Fanny Prezman², Eric Serrano², **Maxime Ryckewaert¹***

¹ITAP, Univ Montpellier, INRAE, Institut Agro, Montpellier, France

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In different disciplines, visible and near infrared spectroscopy (VIS-NIR) is increasingly used for in-line and handheld applications. There is a risk that abnormal observations may occur. It is then important to handle correctly the outliers to develop effective prediction models.

The objective of this study is to examine the potential of a robust method called Roboost-PLSR [2] to improve the performance of prediction models by managing outlier measurements. This work focuses on a case study to predict the sugar content of grape berries from three different *Vitis Vinifera* varieties in a maturity monitoring context.

Hyperspectral images were acquired of grape berries of Syrah, Fer-Servadou and Mauzac varieties. Reference measurements of sugar content were made in the laboratory by densimetric baths. The performances of the RoBoost-PLSR models were compared to the performances of reference models using partial least squares regression (PLSR). The reference prediction criteria obtained using PLSR were: Syrah ($R^2 = 0.971$; RMSE= 5.36 g/L), Fer-servadou ($R^2 = 0.788$; RMSE= 11.69 g/L) and Mauzac ($R^2 = 0.690$; RMSE = 15.61 g/L). Using RoBoost-PLSR models improved the prediction qualities with: Syrah ($R^2 = 0.990$; RMSE=3.14 g/L), Fer-Servadou ($R^2 = 0.848$; RMSE= 10.20 g/L) and Mauzac ($R^2 = 0.927$; RMSE = 7.58 g/L).

The results confirm that the Robust-PLSR method allows a better consideration of outliers in the calibration set, hence improves the overall prediction.

References

1. A. Courand *et al.*, Evaluation of a Robust Regression Method (RoBoost-PLSR) to Predict Biochemical Variables for Agronomic Applications: Case Study of Grape Berry Maturity Monitoring. *Chemometrics and Intelligent Laboratory Systems* 221,104485 (2022).
2. M. Metz *et al.*, A novel robust PLS regression method inspired from boosting principles: RoBoost-PLSR, *Anal. Chim. Acta* 1179, 338823 (2021).

T05. HYPERSPECTRAL IMAGING FOR NON-INVASIVE FISH FRAUD DETECTION

María-José Sáiz-Abajo, Miriam Alonso, Paula Luri and Jaione Echávarri

National Centre for Food Technology and Safety (CNTA). NA 134, Km. 53. 31570 San Adrián, Navarre, Spain.

The harmonisation of methods for the detection of fraud in fish is an important and current issue. The main fraud causes in the fishery industry are origin mislabeling, species substitution and frozen fish sold as fresh. SUREFISH project aims at valorizing traditional Mediterranean fish by fostering the supply-chain innovation and consumer confidence on Mediterranean fish products through deploying innovative solutions to achieve unequivocal traceability and confirming their authenticity, thus preventing frauds. In this context, VIS-NIR hyperspectral imaging (HSI) has been studied as possible techniques to detect some types of frauds in fish being time-saving and allowing analysis without destroying the sample. Two types of fish have been studied: anchovies (*Engraulis encrasicolus*) and bluefin tuna (*Thunnus thynnus*).

In the case of anchovies two different origins were analysed (Mediterranean and Atlantic) in addition to fresh/thawed samples. Two HSI cameras were used in ranges VIS-NIR (400-1000 nm) and NIR (935-1720 nm) to explore both types of frauds. VIS-NIR range is able to capture both type of information (origin and fresh/thawed samples) in anchovies both on the inside part (muscle) or outside (on the skin) whereas NIR range is only able to detect sample origin with high accuracies.

On the other hand, for bluefin tuna, sampling was performed only on the fish muscle. In this case HSI in the VIS-NIR was the most useful spectral range to calculate models able to detect fresh/thawed samples.

Hyperspectral imaging, combined with appropriate chemometric techniques, can generate models able to predict two types of fish fraud: geographical origin and sale of thawed fish as fresh fish, which makes it an effective tool to fight against this type of frauds in the fish industry without the need to destroy or process the sample.

T06. UNSUPERVISED ANOMALY DETECTION IN HYPERSPECTRAL IMAGES OF FRUIT BY ADAPTING A VECTOR QUANTIZED VARIATIONAL AUTOENCODER

Remi Van Belleghem^{1,2}, Bart De Ketelaere¹, Wouter Saeys^{1,2}

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In order to reduce food waste, it is important that the fruit and vegetables that reach consumers are of the highest quality. Hyperspectral imaging has proven to be a promising technique to non-destructively assess the quality of biological products and could therefore help in reducing food waste. To efficiently analyze these hyperspectral images, deep learning methods have recently been proposed. These deep learning methods are typically classification networks that are trained for classifying pixels, pixel patches or even entire images. Although good performance can be obtained, these networks require a large dataset with many examples from all possible defect categories for training the network.

To overcome this challenge, we propose the use of an unsupervised anomaly detection algorithm for online quality control based on encoder-decoder networks. Such networks can be trained with images from good samples only and allow to detect bad quality samples based on the reconstruction errors.

In this study, a Vector Quantized Variational Autoencoder (VQ-VAE) [1] was adapted for hyperspectral image anomaly detection. As a case study, a public dataset with hyperspectral images of avocados at different ripeness stages [2] was used. This dataset contains 59 avocado fruit labeled as unripe, ripe and overripe. The ripe avocados (30) serve as 'good' samples, whereas the unripe (13) and overripe (16) avocados are the 'bad' samples to be detected.

The results show that when using a larger testing dataset, and therefore a smaller training dataset, the autoencoder can achieve similar results compared to the supervised training algorithm. However, when enough training data is available, the supervised approach still outperforms the unsupervised anomaly detection.

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T07. HYPERSPECTRAL-LIDAR FUSION APPLIED FOR MULTITEMPORAL ANALYSIS OF URBAN AREAS

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Multitemporal analysis of an urban environment using remotely sensed data is relevant for scientific research, e.g., monitoring climate change and analyzing the quality of urban materials. An urban area is characterized by a mix of natural and artificial materials constantly changing due to weather conditions or human activities. Therefore, change detection of such an area is a complex challenge that is efficiently approached using hyperspectral (HS) sensors and lidar scanners. While lidar point cloud focuses on geometrical and object changes, HS data define intraclass variability by detecting significant differences in material (Fig. 1).



Fig. 1. Binary change detection map on bitemporal data from 2019 and 2021.

This study presents a general change detection technique based on fused HS (Hypex VNIR-1800 and SWIR-384) and lidar (Riegl VQ-560i) data acquired in 2019 and 2021 over Baerum municipality near Oslo in Norway. This approach requires understanding of physics and is

based on raster segmentation to retrieve the most relevant urban surfaces. In such a segment, HS endmembers and lidar features are extracted as abundance maps to obtain urban surface characteristics. Those abundance maps are fed into a deep learning classifier to analyze urban changes. The validation is carried out on simulated changes defined by user priorities. Such an analysis of urban areas has a great potential to create multitemporal local databases with critical urban surfaces.

T08. HYPERSPECTRAL IMAGING IN NUCLEAR FORENSICS INVESTIGATION

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In the event of a discovery of illicit trafficking of nuclear material, the material type, its manufacturing process and its site of origin must be determined as quickly as possible [1]. Recently an approach for rapid identification of uranium ore concentrate (UOC) powders using colour, textural and hyperspectral imaging (HI) signatures was developed (figure 1). 79 industrial UOC powders were first grouped into six different predefined colour categories, using a supervised colour-based classification model. Scanning electron microscope (SEM) and hyperspectral images were taken of the powders. Machine learning was used to develop sample classification models using either the powder texture captured by the SEM images, or the spectral signature derived from the hyperspectral images. A three-fold cross-validation scheme was used to assess model performance. An average prediction accuracy of 82% and 97% was reached for the textural and spectral-based classification models, respectively.

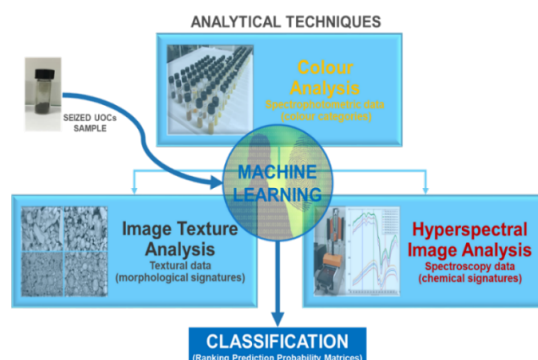


Fig. 1. Combination of different analytical techniques for UOCs powders identification and classification.

The presentation will focus on the results obtained using hyperspectral imaging for characterization and classification of uranium ore concentrate (UOC) samples. Characterization, the modelling approach, preliminary results as well as future challenges and improvements will be addressed. The proposed research will open a new avenue combining physical, morphological and in particular molecular information (this work represents the first application of HI in the nuclear forensic field), for attribution of unknown UOCs powder, potentially enabling rapid identification without comprehensive sample preparation.

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T09. SPATIAL AND SPECTRAL LIMITS OF DETECTION (LOD) IN THE DETECTION OF MICROPLASTICS IN SAND BY NEAR INFRARED HYPERSPECTRAL IMAGING

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Several recent manuscripts point to Near-infrared hyperspectral imaging (NIR-HSI) as a feasible technique to detect microplastics (ranging in size from 0.1 to 1000 microns) in natural samples in real-time [1], [2]. However, there remain a number of questions that must be answered to address analytical concerns related to the interactions between NIR radiation, microplastics, and environmental matrices:

- *Scattering*: Will the spectrum of a pixel containing a microplastic (MP) be affected by the scattering promoted by the environmental matrix? If so, to what extent will this effect change the spectrum relative to the spectrum of the pure plastic?
- *Spatial resolution*: What is the smallest spatial level at which we can be confident that the microplastic signal will still be visible?

- *Spectral resolution*: Is there a combination of wavelengths in the spectra that remain selective for the microplastic?

These questions have been thoughtfully studied in this work. First, microplastics of polypropylene, polystyrene, and acrylonitrile butadiene styrene were characterized by microscopy, and each individual MP was placed on the surface of a separate petri dish filled with sand from a local beach (Plentzia, Spain). Then, NIR-HSI images were collected with a bench-top push-broom NIR-HSI instrument working in the range of 1000–1600 nm at spatial resolutions from 10 to 100 microns.

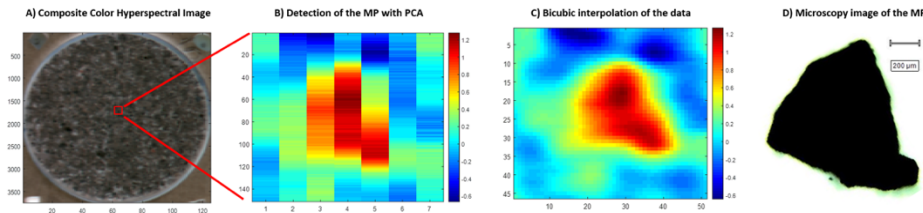


Figure 1: A) Composite Color hyperspectral image. B) Area of the MP. C) Interpolated area. D) Microscopy of the MP.

Figure 1 provides an example of the data processing procedure of an image (Figure 1A) of a polystyrene MP in sand. Principal Component Analysis (PCA) was used to ascertain the presence and position of the MP in the petri dish (Figure 1B). Bicubic interpolation was then applied to the hyperspectral image (Figure 1C) to better understand the spectral signal of the MP. The high similarity between the interpolated information and the microphotography of the MP (Figure 1D) gives credence to the accuracy of the limit of detection calculated.

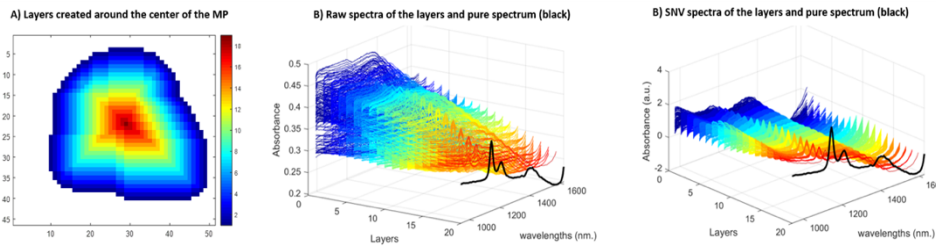


Figure 2: A) Layers of spectra extracted. B and C) raw and SNV corrected spectra, respectively, for each layer.

Assuming that the MP spectra would be “purest” in the middle of the MP, spectra at different radii with respect to the centroid were compared (Figure 2). This showed that the spectra of the MP are less similar to the pure spectrum than expected. Although the scattering decreases and the peak at 1145 nm increases towards the center of the MP, the peaks at 1200 and 1400 nm are completely masked by the influence of the sand.

Additional alternatives to calculate the spatial and spectral Limit of Detection of the different plastics will be presented and thoughtfully discussed.

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T10. USING HYPERSPECTRAL CAMERAS TO DETECT CORROSION PRODUCTS IN EPOXY COATINGS FOR OFFSHORE WIND TURBINES

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Detecting coating defects on offshore wind turbines is a manual, dangerous, and costly process. This inspection method is also subject to interpretation, and quality can vary depending on the inspector's training and experience. Camera-based methods could automate the inspection process, but are also subject to interpretation, as corrosion based only on color and texture information can lead to false positives [1,2,3]. On the other hand, more chemical methods such as XRD, FTIR, and Raman spectroscopy are not suitable for large measurement areas or in situ measurements. Hyperspectral imaging combines high spatial resolution with chemical analysis.

In this study, we investigate the use of hyperspectral imaging (HSI) cameras in the shortwave infrared region to detect coating defects. From previous studies [4], we know that we can identify the different corrosion minerals using SWIR HSI cameras. The large number of spectral bands captured is used to identify specific corrosion minerals that form during the corrosion process, allowing for more accurate and objective classification than RGB images. Several carbon steel samples with highly corrosion resistant, multilayer epoxy coatings were prepared and subjected to the ISO 12944-9 accelerated corrosion test. A test cycle consisted of a salt spray chamber (three days), a freeze chamber (two days), and a UV weathering chamber (three days). Seven cycles were performed to induce corrosion in the specimens.

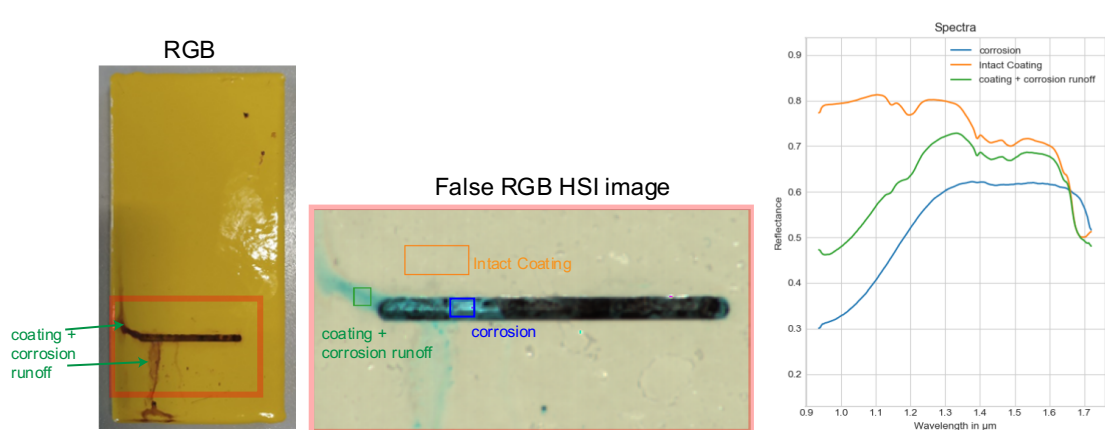


Fig. 1. Left: RGB image. Mid: Close up false RGB image from the hyperspectral cube with annotated squares. Right: Average spectra of the annotated squares. This sample has endured two accelerated corrosion tests.

An analysis of the different spectra shows that it is possible to distinguish clearly between: intact epoxy coating, bare metal, corroded metal (in the form of corrosion minerals) and a mixture of corrosion minerals and coating. The latter looks like corrosion in the visual spectrum, as shown in Figure 1. However, these are deposits of the corrosion products that adhere to the coating and are in no way responsible for the degradation process of the coating. What would be a false positive detection in the visible range is correctly detected with the SWIR hyperspectral camera. In this study, we will give an overview of the corrosion growth and deterioration of the coating detected by the HSI camera in the different cycles. These results will be verified by chemical analysis method such as FTIR and XRD.

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T11. CHARACTERIZING NI-P METALLIC COATINGS USING HYPERSPECTRAL IMAGING IN SHORT-WAVE INFRARED

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In recent years, close-range hyperspectral imaging has obtained valuable achievements in monitoring and quality control of different materials. Hyperspectral imaging collects the reflection of light and splits it up in more than 100 narrow wavelength bands, covering the visible range and beyond, which allows characterizing materials that are visually not distinguishable (same color, texture, etc.). Nickel Phosphor (Ni-P) coatings are extensively employed in engineering, owing to their mechanical and tribological properties which confer protection against corrosion. The chemical properties and the thickness of the metal coating vary depending on the application. Also, for some applications, for example the stripping of defected coatings, it is important to know what is the substrate material under the metal coating. Yet when Nickel coating is applied to different metals, the final look is visually very similar and hence it is not easy to define the type of substrate under it.

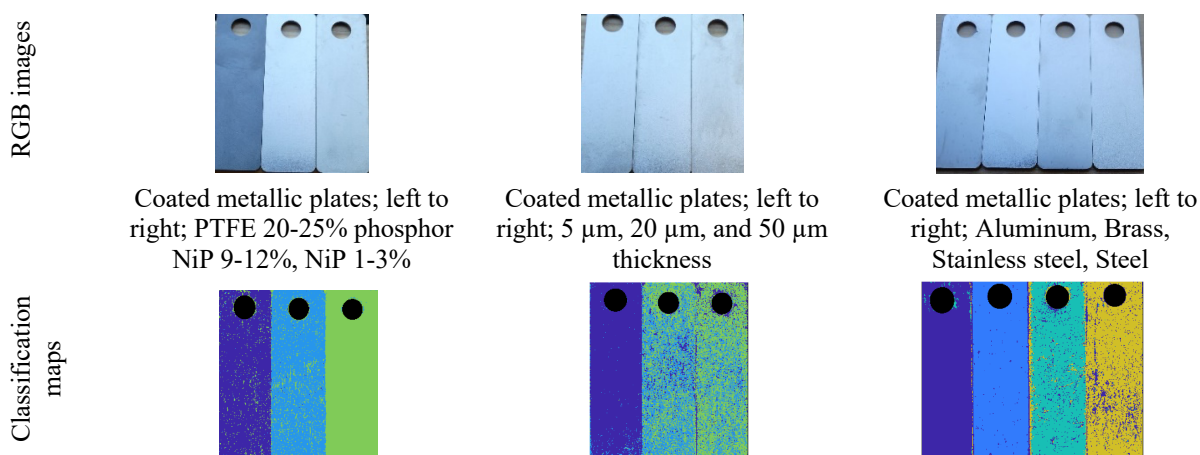


Fig.1. The results of classifying different sets of metallic-coated samples using short-wave infrared hyperspectral imaging

In this study, we investigated the potential of hyperspectral imaging in the SWIR range (using a Specim FX17 camera with a spectral range of 1000-1700nm) to differentiate 3 different sets of samples. The first set of samples contains stainless steel plates with 3 different types of coatings; NiPTFE coating which contains 20-25% PTFE particles, NiP 1-3% and NiP 9-12% coatings which contain 1-3% and 9-12% phosphor respectively. The next set of samples contains stainless steel samples, each coated with NiP 9-12% coating but with 3 different thicknesses: 5 μm , 20 μm , and 50 μm . The last set of samples contains 4 different metallic substrates similarly coated with a 5-micron layer of NiP 9-12% coating. The substrate metals are Steel, Stainless steel, Aluminum, and Brass. Except for the PTFE sample in the first set of samples, the rest of the samples look visually very similar (RGB images in Figure 1). The hyperspectral data were analyzed using a Support Vector Machine algorithm to classify different types of materials within each set of samples. The results (Classification maps in Figure 1) show that hyperspectral imaging in SWIR can be used as a non-destructive testing method for characterizing and classifying metal coatings.

T12. PLASTIC CLASSIFICATION VIA IN-LINE HYPERSPECTRAL CAMERA ANALYSIS AND UNSUPERVISED MACHINE LEARNING

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An increase in the quality of recycled plastic is paramount to address the global plastic challenge and applicability of recycled plastics. A potent approach is mechanical plastic sorting but sufficient analytical techniques are needed. This study applies unsupervised machine learning on short wave infrared hyperspectral data to build a model for classification of plastics. The model can successfully distinguish between twelve plastics (PE, PP, PET, PS, PVC, PVDF, POM, PEEK, ABS, PMMA, PC, and PA12) and the utility is further proven by recognizing three unknown samples (PS, PMMA, PC). The experimental setup is constructed similar to an in-line industrial setup, and the machine learning is optimized for minimal data processing. This ensures the industrial relevance and is a stepping-stone to solve the global plastic challenge.

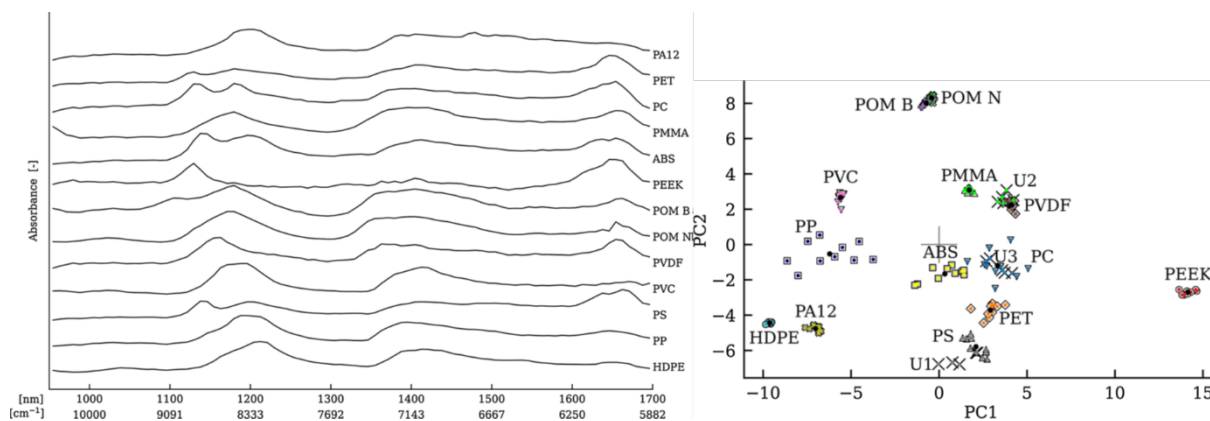


Fig. 1. Obtained plastic spectra from the hyperspectral camera (left) and the score plot (right).

In the score plot in fig. 1 (right) the color defines the assigned material class and the unknown materials U1 (weighing boat), U2 (safety glasses) and U3 (transparent plastic sheet) are all correctly classified.

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T13. HSI-NIR FOR THE QUANTIFICATION OF COLLAGEN IN BONES: HOW CHEMICAL MAPPING CAN HELP IN PRESERVING ARCHEOLOGICAL FINDS

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Many rarest bones and human remains in Prehistory are much too precious and considered a cultural and historical patrimony, and so the application of destructive methods -such as ¹⁴C- must be as limited as possible. The identification and quantification of collagen in archaeological bones play a crucial role in the ¹⁴C dating protocol because a significant amount of proteins (1% yield of collagen)¹ is requested for performing a reliable radiocarbon analysis. The advantages of the HSI-NIR technology can be of high impact in this

context, in particular regarding the non-destructiveness and the possibility to map, from a spatial extent, the area of the bone in which the proteins are more present. A first milestone in mapping collagen in bones by means of HSI-NIR was achieved by the authors², applying the NDI approach to few archaeological samples. Acting upon this, a quantification model is now proposed thanks to the analysis of 60 archaeological bones, ranging back from the modern age to more than 50,000 years ago. For the development of the PLS regression model, NIR images of both bone powders and fragments were acquired in the spectra range 1000-2500 nm (Specim SWIR 3 camera) and then the samples were submitted to collagen extraction at the BRAVHO ¹⁴C lab, following the procedures of Talamo et al. 2021¹. With a RMSECV of 2.2% wt, the proposed strategy was applied to unknown samples demonstrating how HSI-NIR can be a sustainable pre-screening method to quantify the presence of collagen on bone samples in a non-destructive way.

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T14. COMPARISON OF REFLECTANCE FTIR, VNIR AND SWIR SPECTRAL IMAGING FOR THE DISCRIMINATION AND IDENTIFICATION OF BACTERIAL SUSPENSIONS DRIED ON STAINLESS STEEL

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It is of critical for the food industry to take appropriate measures to monitor and prevent the occurrence of microbial contamination during food preparation. This work investigates non-contact reflectance spectral imaging techniques, i.e. microscopic Fourier transform infrared (FTIR) imaging, macroscopic visible-near infrared (VNIR) and shortwave infrared (SWIR)

spectral imaging and for microbial characterization/identification on stainless steel. Spectral images of two gram-positive i.e., *Bacillus subtilis* (BS) and *Lactobacillus plantarum* (LP) and three gram-negative i.e., *Escherichia coli* (EC), *Cronobacter sakazakii* (CS) and *Pseudomonas fluorescens* (PF), bacteria were collected from dried suspensions of bacterial cells dropped onto stainless steel surfaces. Classification models were built on either mean spectra from a dried drop of bacterial suspension (“object level classification”), or from pixel spectra obtained after masking the image background (“pixel level classification”). Classification models were developed at an object and pixel level to compare the capability of the studied techniques for classification between gram positive or gram negative (GP/GN) samples, classification between the gram positive samples (BS/LP) and classification between the gram negative samples (EC/CS/PF). Through the use of independent biological replicates for model validation and testing, FTIR reflectance spectral imaging was found to provide excellent GP/GN classification, with accuracies on the independent test set exceeding 99 %, excellent classification between GP species and poorer accuracy for classification between GN species. Excellent classification accuracy was obtained for GP/GN classification when VNIR-SWIR data were fused together; while poorer accuracies were found for classification within the GP species and GN species.

T15. DETECTION OF CRONOBACTER SAKASAKII BIOFILMS ON ALUMINIUM COUPONS THROUGH ULTRAFAST FTIR SPECTRAL IMAGING

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Microbial contamination is a threat to human health, associated to regular disease outbreaks throughout the world and holding important environmental and economic repercussions. Most foodborne diseases are due to biofilm forming microbes. These bacteria bind to surfaces, imbedded in a protective extracellular polymeric matrix. Detection of biofilms in food related surfaces is thus critical for early detection of microbial contamination in food industries. This work explores the applicability of FTIR imaging to detect *Cronobacter sakazakii* biofilms on aluminium coupons. Biofilms were grown at room temperature in a

dynamic bioreactor for 24 hours. Five replicates of control and biofilm coupons were analysed. Principal component analysis (PCA) of mean spectra (680 to 5000 cm^{-1} at 16 cm^{-1} spectral resolution, 1 scan per point) was able to distinguish between control and biofilm coupons (for 4 out of 5 cultured coupons). The spatial variability of biofilm formation within coupons was studied on the projection of pixel spectra (200 μm per pixel) on the PCA space (Figure 1). These results show the feasibility of using ultrafast FTIR scanning for the detection of biofilms on aluminium surfaces. High spatial variability was observed within biofilm cultured coupons, pointing out the benefits of using an imaging approach that privileges high spatial resolution over high spectral quality. Further work, including a higher number of samples and biofilms from different bacteria strains would be necessary in order to validate these results and expand this approach towards biofilm identification.

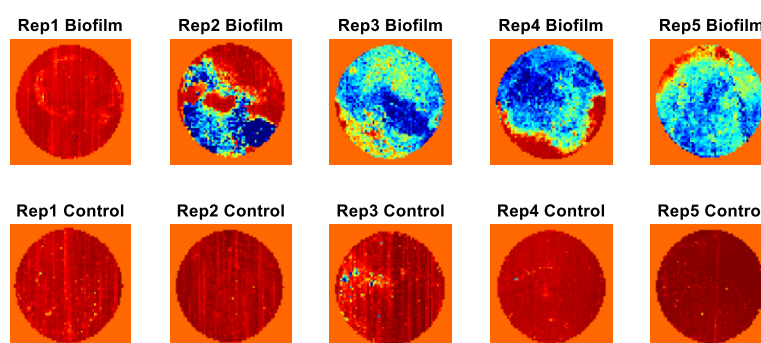


Fig. 1. 1st principal component scores (60.2% variance) of PCA computed on mean spectra per coupon (2nd derivative spectra, 15 window, 3rd order polynomial), projected onto pixel spectra.

T16. IN-LINE IDENTIFICATION OF PB-BASED ADDITIVES IN FISHING ROPES AND NETS FOR RECYCLING WITH HYPERSPECTRAL IMAGING AND MACHINE LEARNING

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Recycling fishing ropes and nets are primordial to overcome the global sea plastic challenge. However, the recycle from fishing ropes and nets can be contaminated by unwanted or banned additives, i.e., Pb-based pigments. Consequently, they will contaminate the whole recycled batch, if these contaminants are not identified and excluded prior to recycling, yielding the end products worthless. This study utilize an industrial hyperspectral imaging

system and unsupervised machine learning using Vis-NIR data for the identification of unwanted pigments in fishing ropes and nets plastic waste. The model can successfully distinguish between the pigments and identify the challenged pigments in plastic samples.

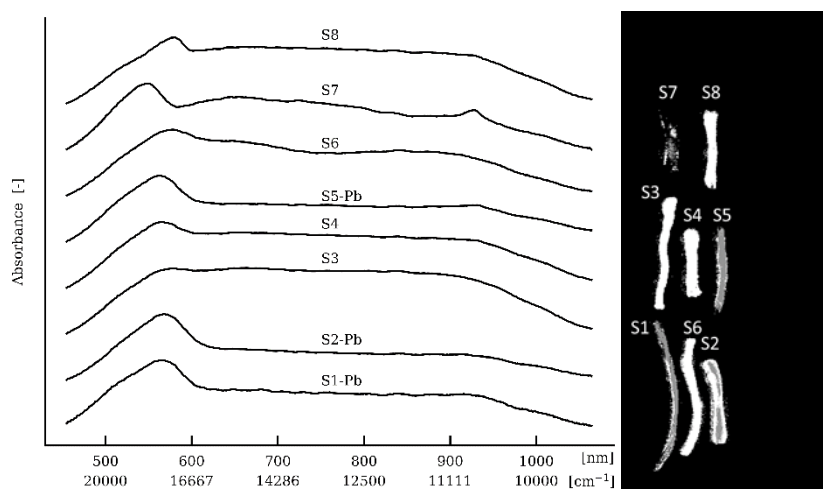


Fig. 1. The hyperspectral Vis-NIR spectra (left) and the Pb-pigment identification of the fishing ropes and nets plastic samples (right).

Examples of the measured spectra (Fig. 1, left) of the fishing ropes and nets plastic samples from 450 nm to 1050 nm. The spectra are used to assign the pigment class (Fig. 1, right), where white and grey represent uncontaminated and contaminated, respectively. The samples S1, S2, and S5 are all correctly classified as Pb-contaminated.

T17. CHARACTERIZATION OF MICROPLASTICS IN MUSSELS USING NEAR INFRARED HYPERSPECTRAL IMAGING

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Microplastics (MPs), defined as polymeric particles with size below 5 mm, are ubiquitous pollutants encountered in all planet ecosystems and across all trophic levels. Mussels as filter feeders are capable to accumulate particulate matter, and ingestion of MPs by mussels is well

documented. Hence this organism was proposed as an indicator species for MP contamination in seawater.

The objective of this work was feasibility study of the NIR Hyperspectral imaging for identification of particles extracted from mussel tissue. Mussel *Mytilus spp.* specimens were collected in January and February of 2019 from four natural banks in the Portuguese coast. After soft tissues digestion using alkali (KOH) and filtration, particles that presented no cellular or organic structures visible inside and kept the structure when prodded were counted as potential MPs. NIR hyperspectral images of the visually sorted particles arranged on the microscopy slides were recorded using a benchtop HSI system (FX17e HyperSpectral LabScanner, Specim, Finland) in the wavelength range 900–1700 nm with spatial resolution 17 μm . MPs identification was done using FT-MIR spectroscopy. ROIs corresponding to the individual particles were identified in the pre-processed NIR images by analyzing false color images and using optical microscopic images as a reference. Geometrical parameters and mean spectrum of each particle were computed. The PLS-DA classification models were developed using extracted spectra and MPs identification obtained by FT-MIR as a reference. This study confirmed potential of NIR imaging as a rapid MPs' identification tools highlighting importance of reference materials for the characterization of MPs in the environment.

Acknowledgments. We acknowledge financial support to CESAM by FCT/MCTES (UIDP/50017/2020+UIDB/50017/2020 + LA/P/0094/2020) and to CIIMAR (UIDB/04423/2020 + UIDP/04423/2020), through national funds, and through the strategic project ALG-01-0145-FEDER-032453.

T18. PARSKETCH-PLSDA, A METHOD TO HANDLE LARGE AMOUNTS OF DATA GENERATED BY HYPERSPECTRAL IMAGING: APPLICATION TO SUNFLOWER GENOTYPE DISCRIMINATION

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The use of optical instruments such as NIR spectroscopy or hyperspectral imaging is increasing, offering the possibility to generate large amounts of data automatically. However, the large amount of data, often called massive data, leads to difficulties in managing and analysing it. Processing this massive amount of spectral data is a challenge.

Recently, a method called ‘parSketch-PLS’ has recently been proposed [2] to implement a local approach to a large volume of spectral data. This method combines a fast neighborhood search method (parSketch) with PLS. This method is valid to predict categorical variables by adding a Discrimination-Analysis (DA) step like PLS with PLS-DA.

In this presentation, we propose to compare parSketch-PLS-DA with the reference method PLS-DA in a context of varietal discrimination. For this purpose, a spectral database was formed by collecting 1,300,000 spectra from hyperspectral images of leaves of four different sunflower genotypes.

Results show that the prediction model obtained by PLS-DA has a classification error close to 23% on average across all genotypes. ParSketch-PLS-DA method outperforms PLS-DA by greatly improving prediction qualities by 10%.

These results are encouraging and allow us to anticipate the future bottleneck related to the generation of a large amount of data from phenotyping generating complex structures and non-linear relationships.

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T19. CORRECTING TIME-INDUCED MEASUREMENT EFFECTS IN NIRS MODEL: APPLICATION TO THE EARLY DETECTION OF “EARLY BLIGHT”

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Spectroscopy and hyperspectral imaging (HSI), especially in the visible and near infrared (VIS-NIR) domain are very popular automated and non-destructive techniques for the detection of numerous plant pathologies [1]. Indeed, with the appropriate analysis and modelling methods, it is possible to discriminate infected plants from healthy ones, to predict infection levels and stages, or even to discriminate between different diseases [2–5].

Although there are some examples in the existing literature, early detection remains a challenge [6]. Indeed, the changes in signals induced by the infection at early stages can be occulted by important variabilities. Some variations can be reduced or corrected by ensuring stable measurement environments and controlled growing conditions. However, plant-pathogen interaction remains a dynamic process, and healthy plants themselves are subject to uncontrolled natural physiological fluctuations. In this article, it is proposed to consider the time induced variabilities, within the modelling process in order to improve their robustness and performances of discrimination between healthy and infected plants. The problem is addressed with the case study of the monitoring of potatoes' early blight (*alternaria solani*) during the first hours after infections (HAI). The purpose of this article is to investigate three practical correction methods of the time induced measurement effects and to compare them with the reference method PLSDA (Partial Least Square Discriminant Analysis):

- a) predicting the health status and the HAI time-points altogether within a PLS2 model
- b) predicting health status after internal linear correction ([7]) with a time constraint PLS2
- c) predicting health status with EPO-PLSDA considering time (external parameter orthogonalisation - partial least square [8])

Eventually, early blight can be detected 36h after inoculation for six different varieties of potatoes with an average accuracy above 75% when the reference method cannot achieve reliable predictions. Know resistant varieties such as "Aracy" are however not properly modelled. The proposed method could be extended into a more generic framework of correction.

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T20. CHARACTERIZATION OF N-DOPED DIAMONDS AFTER ELECTRON BEAM IRRADIATION BY INFRARED SPECTRAL IMAGING

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Nitrogen is the most common atomic impurity found in both natural and synthetic diamonds. It may lead to different lattice defects. Most synthetic diamonds prepared by the HPHT method (high pressure high temperature) are type Ib diamonds, which contain single neutral nitrogen atoms at various lattice positions (called N^0 centers). Irradiation of such diamonds with electrons may partly convert N^0 centers into positively charged single nitrogen atoms (N^+ centers). Both N^0 and N^+ centers may be inhomogeneously distributed within a diamond sample. Since both types of defects show specific vibrational modes in the IR spectrum (N^0

at 1344 cm^{-1} , N^+ at 1332 cm^{-1}), the conversion from one type to the other may be studied by infrared spectroscopy.

In the present study, various synthetic diamonds with dimensions in the order of a few millimeters were irradiated by an electron beam from a 7 to 10 MeV electron accelerator (MEVEX, Canada). Before and after irradiation, samples were analyzed by spectral imaging using an IR microscope equipped with both a FPA and a single element MCT detector in order to highlight both the changes induced by the electron beam as well as the distribution of N^0 and N^+ centers across the diamond. In order to characterize the complete diamond surface, it was successively scanned by a raster of FPA images leading to a final data set of several 10^5 spectra. This approach is particularly useful for the characterization of diamonds, which were not irradiated homogeneously, but with different doses at different positions (e.g. using a mask). Spectral imaging visualizes the degree of conversion from N^0 to N^+ in both irradiated and non-irradiated zones (induced e.g. by electron scattering). Moreover, absolute concentrations of both defects were calculated from relations reported in the literature. In case of N^0 , good correlation with data from EPR measurements was found (N^+ is EPR inactive) [1]. In some cases, also the formation of H1a centers related to nitrogen interstitials in the diamond lattice was observed by means of the formation of a band at 1450 cm^{-1} , which is accompanied by a color change of the diamond to purple.

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T21 SPECTRAL IMAGING AS A TRANSFORMER OF THE FOOD-AG INDUSTRY

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LED spectral imaging systems is a mature technology for a very rich and versatile analysis of food and agricultural products. When used together with cloud databases of images and quality traits it allows for an elegant handling of phenotypic variability as well as process variability, and machine learning models can be created, validation, updated, and deployed in an effective and efficient way. We will present examples of quality testing in seed and grain including purity, damages, and mycotoxin detection as well as examples of powder quality and food authenticity assessment.

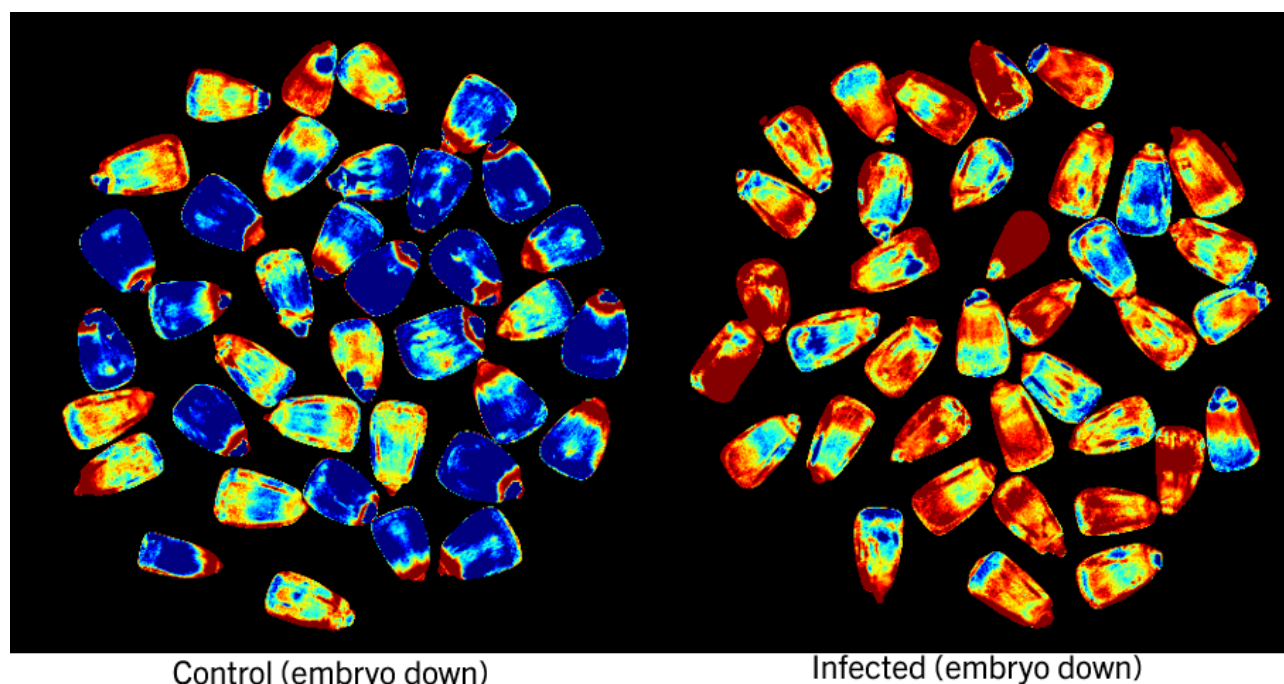


Fig. 1. Healthy (left) and aflatoxin contaminated (right) corn. Score image for nCDA spectral signature.

The multivariate analysis technique, normalized canonical discriminant analysis (nCDA) is used to optimize the application performance as well as to get information about the data/noise structure and importance of specific spectral ranges. The performance is illustrated on a number of real applications on contaminant detection in different materials. More examples and publications are found in [1].

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T22. ONE-STEP CALIBRATION OF INDUSTRIAL HYPERSPECTRAL CAMERAS

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Hyperspectral imaging is gaining interest as an inline reflective analytical technique. The raw data is often applied for classification or process adjustments. Proper calibration can eliminate the background, noise, and artefacts. Further, it enables determination of area fractions and, via spectral information, chemical analysis. This paper demonstrates a simple, robust, and easy-to-operate calibration device for inline calibration of hyperspectral cameras (CMOS and InGaAs) in the range from 450 nm to 1840 nm. The design is flexible,

made from easy sourced materials, and can be adapted to most laboratory and industrial setups. Calibration of intensity, spatial and spectral information is combined in one device and is done in a single pass. Device alignment and subsequent image analysis provides a fast and easy calibration routine for hyperspectral cameras.

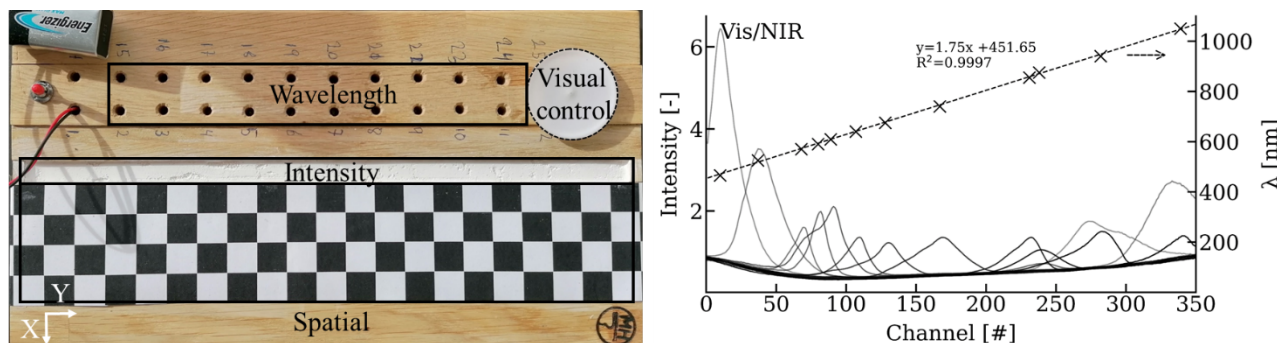


Fig. 1. Photo of calibration device (Left) and wavelength calibration for CMOS sensor (Right).

Fig. 1 shows the calibration board and the data and calibration for the CMOS based on LED's. The total calibration includes intensity, dead pixel, spatial and spectral calibration. All collected on a single device and fully automate parameter extraction is performed via a computer program (Python script).

T23 SEARCHING FOR EXOTIC PIXELS IN LARGE HYPERSPECTRAL IMAGING DATA SETS

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The production of global data in the world is expanding at an astonishing pace. Indeed the amount of data in the world is estimated to be 120 zettabytes at the dawn of 2023. By 2025, the amount of data generated each day is expected to reach 0.5 zettabytes globally. We are all witnessing this evolution in our research and more particularly in the field of hyperspectral imaging. Indeed, the development of new instrumental concepts and new experimental methodologies allow us today to acquire data sets containing up to several million spectra acquired on a single sample. Thus chemometrics tools have never been more valuable for exploring such data sets. However, our analytical objectives have not changed in the face of these new data structures. Indeed, we still want to propose an exhaustive exploration highlighting the presence of both major and minor compounds and even traces.

We can even say that the latter are often the most interesting to detect because we are potentially unaware of their presence, which is of course not the case for the major compounds. The main problem is that minor compounds are often present on a small number of pixels representing a very small variance in the spectral data set. The majority of chemometric algorithms exploiting the concept of expressed variance do not allow the detection of these compounds, especially since the signal-to-noise ratio is often limited in spectroscopic imaging. Based on the principle that a spectrum is a point in a multidimensional space, an imaging data set is a point cloud contained in a hypervolume, its surface being called convex hull. In the context of spectroscopy, it is shown that the spectra present on this surface are potentially the purest ones in the data set explored, the spectra within the volume being linear combinations of these specific spectra. Ghaffari *et al.* have elegantly exploited this concept in the signal unmixing framework by proposing the extraction of so-called *Essential Spectral Pixels (ESPs)* [1]. We propose here a new strategy called *Interesting Features Finder (IFF)*, which seems to be more suitable for noisy data. It is based on the projection of the dataset on a very large number of random vectors for the selection of pixels of interest present on the convex hull taking into account their selection frequency. Various datasets will be used in this work to show the potential of our approach.

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T24. AUTOMATIC PARASITE DETECTION IN FISH USING HYPERSPECTRAL IMAGING

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Manual inspection of fish fillets is a huge bottleneck for the industry, accounting for significant share of the production cost and also reducing the processing speed. In this presentation we will show how hyperspectral imaging can be used to automate the quality control to detect parasites (nematodes), hence reducing the manual labor required, reducing the cost and increasing the end product quality [1].

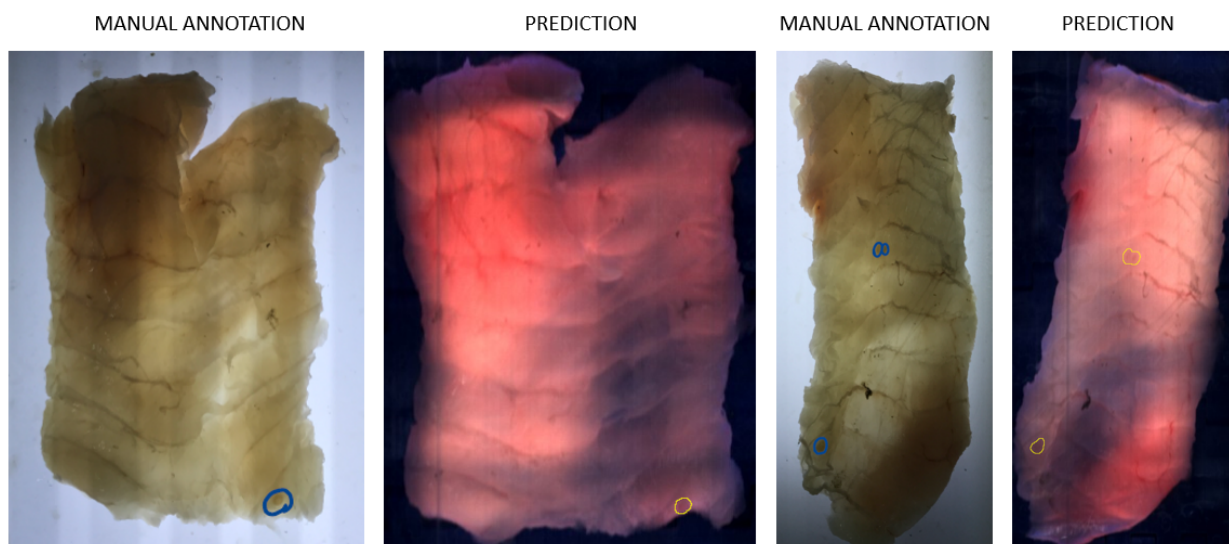


Fig. 1. Regular color images of fish filets on a light table used for manual inspection, and images captured using a hyperspectral camera showing the predicted image and identified parasites

Hyperspectral imaging has been successfully implemented in the *Maritech Eye* system (Maritech Systems AS, Molde, Norway) as a method for automatic and real-time nematode detection in fish fillets moving on a conveyor belt [2]. Using a combination of data analysis methods that use both the spectral and spatial information in the HSI data, an accurate and fast detection of nematodes can be achieved.

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T25. QUANTITATIVE ANALYSIS OF HYPERSPECTRAL IMAGES: SOME NEW INSIGHTS

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When quantitative information is extracted from hyperspectral images, both spatial and chemical information come into play. Although most quantitative analysis methods start by taking mean or median spectra of calibration images to be regressed against their related bulk image concentration, the model established can be used to provide bulk concentrations of unknown images or individual pixel concentrations. In the latter case, the concentration

maps display the spatial distribution of compounds and, hence, the sample heterogeneity [1].

Multivariate calibration methods serve the purpose of quantitative image analysis, but only maps of known analytes can be obtained. Instead, Multivariate Curve Resolution (MCR) gives a complete description of all compounds in the image and, when bulk image concentrations are available, furnishes absolute concentration estimates at an image and at a pixel level [2]. Up to now, quantitative analysis based on MCR is applied as an external step using the information in the resolved distribution maps [3]. A step beyond is incorporating the quantitative calibration model in the iterative MCR optimization, through an image-dedicated version of the area correlation constraint to improve the accuracy in MCR solutions and, hence, the concentration estimates.

The active use of sample heterogeneity information can also improve image calibration models. Actually, using a single mean or median spectrum per calibration image reduces the representation of a sample imaged to a single spectral form and ignores sample heterogeneity. Variographic analysis can help in this context by providing an estimate of the extent of the spatial correlation within an image [4]. Once this is known, several spectra to represent each calibration image can be obtained using mean or median of spectra associated with non-overlapping image areas with a size exceeding the spatial correlation range determined. Working in this way, calibration images will be better defined and a faithful representation of the image variability will be taken into account in the calibration model.

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T26. RECENT ADVANCES IN HIGH-RESOLUTION HYPERSPECTRAL SNAPSHOT COMPUTED TOMOGRAPHY IMAGING SPECTROMETER

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This work details the recent advances in the snapshot hyperspectral computed tomography imaging spectrometer (CTIS) made through the collaboration between Newtec Engineering and the University of Southern Denmark. A CTIS system reconstructs hyperspectral images through the inversion of the linear imaging equation governing the system.

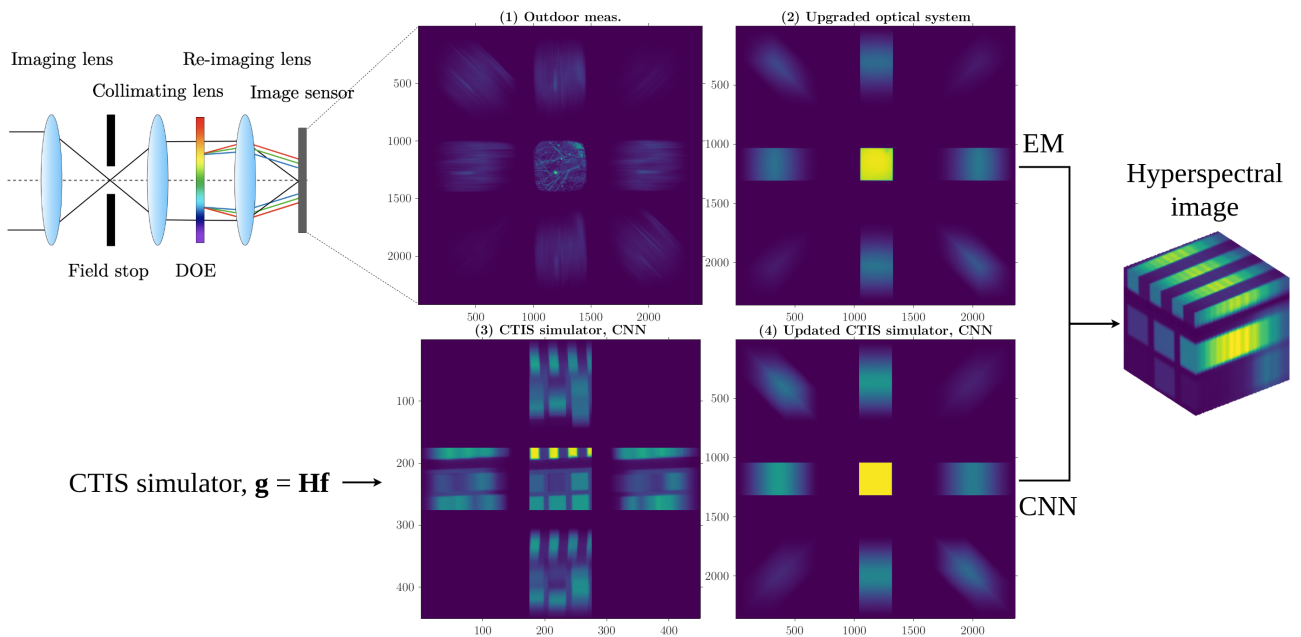


Fig. 1. Overview of the recent advances in CTIS including (1) outdoor measurements, (2) the upgraded optical system, (3) the CTIS simulator and CNN reconstruction of simulated CTIS images and (4) the updated CTIS simulator and reconstruction of true CTIS images. A schematic of the optical layout used in the CTIS system is shown on the left and a reconstructed hyperspectral image using either EM or CNN on the right.

The recent advances (Fig. 1) cover outdoor high-resolution hyperspectral CTIS measurements of fake and real apples in apple trees [1], where a 456x471x417 hyperspectral image covering 438—740 nm was reconstructed using a sparse

implementation of the expectation maximization (EM) algorithm. Subsequently, the optical setup and the system matrix have been upgraded, resulting in improved reconstructions. However, the reconstruction times are limited by the large system matrix, which inhibits real-time reconstructions. To overcome these limitations, CTIS reconstructions of ideal simulated CTIS images using convolution neural networks (CNNs) were proposed for 100x100x25 hyperspectral images with superior reconstructions and lower reconstruction times of ~ 10 ms [2]. The latest development consists of reconstructions of true CTIS images with CNNs trained on simulated CTIS images accounting for the upgraded optical system and system matrix, which show improved performance while maintaining fast reconstruction times.

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T27. COMPARISON OF STRATEGIES FOR PIXEL SELECTION FOR SINGLE- AND MULTI-BLOCK IMAGE MODELING

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When building models on hyperspectral images, one of the problems most frequently encountered is the large amount of data involved, which can in turn result in long computational times if not severe memory requirements. In particular, since normally such problems arise from the spatial dimensions, a possible solution could be to select subset(s) of pixels to be used for further model building. In this context, the number and identity of the pixels to be used could have a significant impact on the performances of the models built.

In the present communication, different possible approaches for selecting subsets of pixels for further model building will be considered both in the case of a single block of data and for image fusion (or multi-block image modeling in general, as it can result from preprocessing fusion strategies).

T28. SPARSE NON-NEGATIVE MATRIX FACTORIZATION OF HYPERSPECTRAL IMAGES DOWN TO ESSENTIAL PIXELS

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Hyperspectral imaging combines the benefits of microscopy and spectrometry, by simultaneously collecting spatial and spectral information. This property makes HIS invaluable for e.g. food quality control, pharmaceutical process control, plastic sorting, and biological measurements. However, HS Images are enormously large to handle and store, which is challenging in applications where analysis time has top priority [1]. Methods to reduce analysis resources in HSI are therefore essential for high-throughput applications.

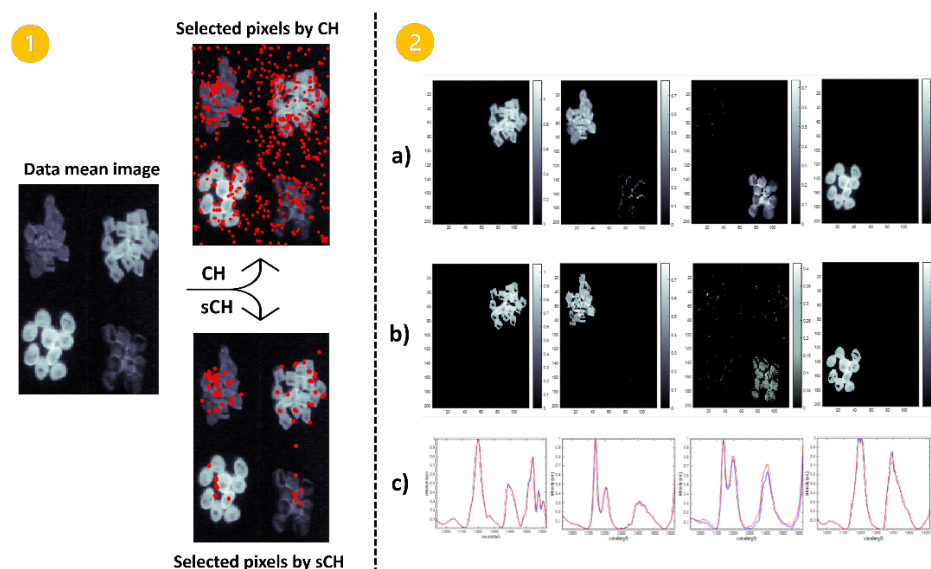


Fig. 1. The difference between CH and sCH is presented in part 1. The results of Sparse-NMF on the full/reduced data are shown in part 2.

Sparse Non-negative Matrix Factorization (Sparse-NMF) can help to recover the “pure contribution maps/spectral profiles” of the components to seriously speed-up analysis of the essential information rather than the full image. A strategy is introduced which recovers the most informative part of the bilinear data sets using the boundary of the data in PCA space defined by a Convex Hull (CH) [2]. Figure 1 presents the mean image of HSI data which contains four types of plastics. Using CH will help to recover the most informative pixels of HIS as is shown by red dots in figure 1. To avoid pixel selection from the background, image segmentation is implemented before applying CH. As it is present in figure 1 the selected pixels by sCH (segmentation + CH) are more convenient. This allows Sparse-NMF to provide analysis results comparable to those of the full image, with less than 1% of the available

data (figure 1). This greatly reduces analysis times, which greatly increases the potential throughput of e.g. smart conveyor belts that use HSI, and requirements to store HSI data to recover chemical information.

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T29. TOMOGRAPHIC RECONSTRUCTION OF HYPERSPECTRAL IMAGES - A HYBRID APPROACH USING CNNs AND THE EM ALGORITHM

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The computed tomography imaging spectrometer (CTIS) is a snapshot hyperspectral imaging (HSI) technique that diffracts spectral information of a scene onto a 2D image. Though, to extract the HSI information a reconstruction is needed. Current methods utilize iterative algorithms such as expectation maximization (EM), but lead to long reconstruction times and moderate accuracy. This work details the recent advances in utilizing CNNs to perform this reconstruction [1]. Our method features superior reconstructions and faster reconstruction time. See Fig. 1 for a performance comparison. These advances emerge through the collaboration between Newtec Engineering and the University of Southern Denmark.

We produce training data by creating a simulator, that allows simulation of CTIS images (Inputs) based on hyperspectral images (Outputs). Our simulator accounts for the illuminant, diffraction efficiency of the diffractive optical element, as well as including a point-spread function and noise. Furthermore, we've investigated different network types, as well as a hybrid approach that combines a sparse expectation maximization algorithm

with a CNN. Throughout this, a thorough investigation has gone into testing different architectures including the U-Net [3].

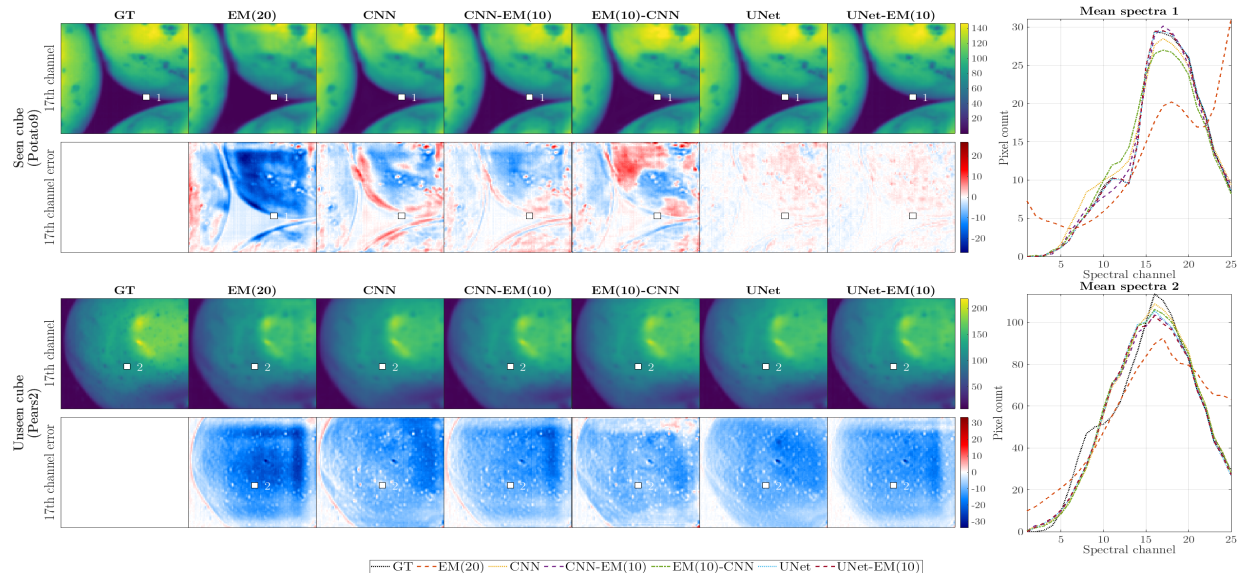


Fig. 1: Performance comparison plot for (25-channels) reconstruction methods of seen (included in training) and unseen (excluded from training) data, from [2].

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T30. JOIN DATA POLYTOPE ANALYSIS OF MULTIMODAL HYPERSPECTRAL IMAGES

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Hyperspectral images provides both spectral and spatial information of an analytical sample [1]. However, each spectroscopic scheme monitors specific compound classes. So, incorporating multiple spectroscopic techniques helps to support a vast variety of chemicals and this may support us better interpret, describe and discuss the problems at hand [2]. Although a wealth of information can be obtained by combining data sets from different sources, the first issue is to overcome the dramatic size in such data and the second issue is to generate accurate and precise decomposition [3]. Very recently, it was shown that a polytope of chemical images with the support of a convex hull contains all the essential information to retrieve the whole data space (see fig.1) [3].

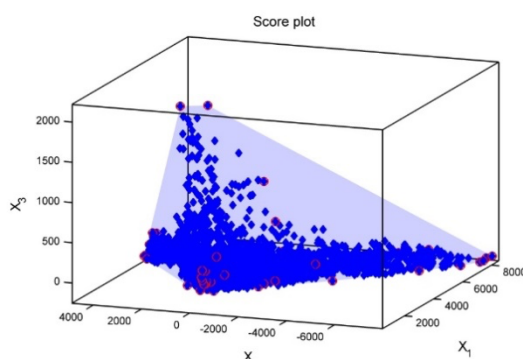


Fig. 1. Microstructure of a hypothetical hyperspectral images. The data cloud enveloped by a polytope was marked in red circles.

In this contribution, joint analysis of data polytopes coming from various spectroscopic schemes is expected (e.g. RAMAN and fluorescence). Such polytope hybridization rather than raw data augmentation resulted in a drastic decrease in the computational time and space required for predictions with similar quality as performed on the full datasets. The advantages can be further attributed to the direct link between original and reduced data, and ease of model exploration. The proposed strategy is evaluated on both simulated and real experiments.

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T31. MULTI-SPECTRAL REFUSE SEGMENTATION FOR REFUSE SORTING SYSTEMS

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The ever-changing refuse composition motivates automated refuse sorting systems that dynamically adapt machine parameters on the fly. State-of-the-art deep learning-based computer vision methods like Convolutional Neural Networks (CNN) have a high demand for annotated data. To greatly reduce the burden of manually labeling mixed-refuse data, we acquire datasets for each waste class separately to synthetically generate mixed-fraction images by combining random mono-waste segments. See Fig. 1 for an overview of our method.

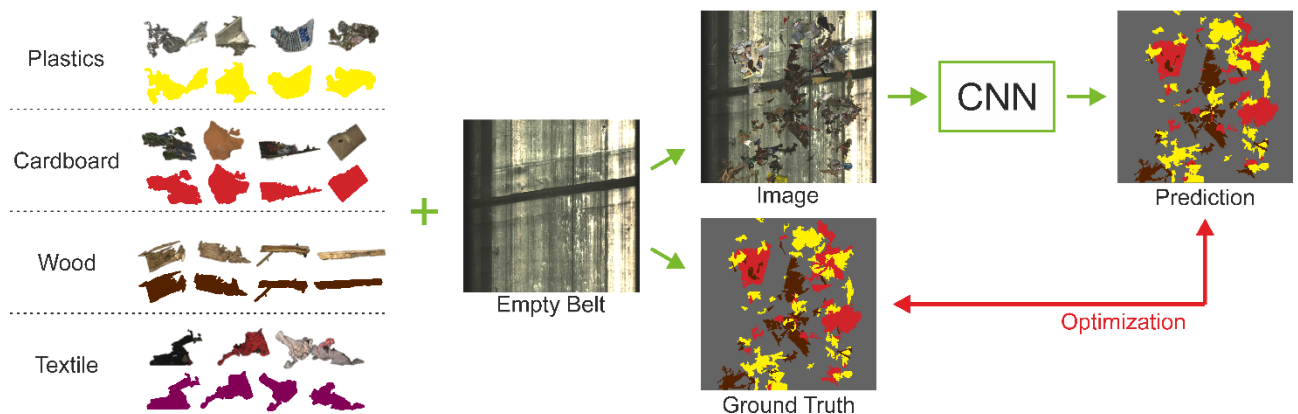


Fig. 1. Method overview. Mono-waste segments are synthetically combined and used for training.

For the automated estimation of refuse composition, we built a system that acquires 4-channel multi-spectral data (RGB+NIR) [1]. We use a DeepLabV3-Plus [2] model for semantic segmentation, which we fine-tune to predict a fraction-specific label from the 4-channel multi-spectral data. In our experiments on synthetic data our method achieves a Dice score of 81.1% (belt 99.1%, plastics 75.8%, cardboard 62.7%, wood 88.6%, textile 79.2%).

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T32. MATHEMATICAL NUANCES OF GENERALIZED LEAST SQUARES. A DESPISED MODEL?

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Generalized Least Squares (GLS) has been used in what is called “Target Anomaly Detection” for several years [1]. Despite its very well demonstrated ability to detect pieces of information on hyperspectral images whose variance is minimal in the variable space, GLS is still not as popular as other methodologies (like classification methods or Multivariate Curve Resolution). The reasons for that might be the lack of a detailed explanation of the mathematical background behind it or the preference for other more well-known methods. This talk will show the mathematical nuances of GLS, comparing it to common approaches in the literature. This comparison will be done by showing real cases (with Raman and Near Infrared hyperspectral Images), which will demonstrate great utility of GLS especially in cases where the alternative methods fail at different levels.

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P01. IN-LINE MONITORING OF FINISHING AND LAMINATION PROCESSES OF BLACK TEXTILES BY NIR HYPERSPECTRAL IMAGING

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Spectroscopic methods such as NIR spectroscopy and NIR hyperspectral imaging have been shown to have an immense potential for applications in process control in textile processing [1]. All previous studies were carried out with textiles with bright colors such as white, beige, light grey etc., that is, with rather high reflectance. In contrast, black materials (which are widely used in technical and other applications) pose a great challenge for analytical methods based on optical reflection due to their very low reflectance and the resulting very low signal intensities. In this study, we demonstrate the use of hyperspectral imaging for in-line monitoring of the state of black materials in various textile converting processes.

Black textile laminates are widely used for interior design in automotive engineering. They consist of one fabric as top layer and another component, mostly a nonwoven, which are bonded to each other with a hot-melt adhesive. For process control, it is required to monitor the thickness and the homogeneity of the hidden adhesive layer during the lamination process. It was shown that the application weight can be determined with a prediction error (RMSEP) of about 6 g/m² regardless of the surface weight of the top layer fabric (120 to 175 g/m²). Moreover, lamination defects (e.g. missing adhesive) can be clearly detected.

Another example is the finishing of black textiles with functional agents such as flame retardants by impregnation in aqueous solutions or dispersions. The objective of process monitoring is directed toward the application weight and the distribution of the agent, but also toward the residual water content of the textile after drying. In the latter case, RMSEP was found to be ca. 0.5 wt%, which is completely in line with the error obtained for comparable bright textiles [3].

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P02. COMPARISON OF A NIR CAMERA AND A NIR MULTIPLEX SPECTROMETER SYSTEM FOR IN-LINE MONITORING OF TEXTILE FINISHING PROCESSES BY HYPERSPECTRAL IMAGING

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Spectroscopic techniques such as NIR spectroscopy and NIR hyperspectral imaging were reported to have a huge potential for monitoring of textile converting processes such as finishing, lamination, cleaning, drying etc. [1]. In this work, we compared two imaging technologies for their suitability for in-line monitoring of the finishing of polyester fabric to be used as ply in tires with an adhesion promoter for rubber (a mixture of a resorcinol formaldehyde latex with an aqueous dispersion of a copolymer of styrene, butadiene and 2-vinylpyridine). Such materials are commercially produced and converted as wide webs with widths of several meters. It was the objective to control the application weight and the residual moisture content after drying with respect to both the corresponding quantitative amounts and homogeneity of the distribution. In the past, NIR cameras have been shown to be powerful tools for the control of textile finishing processes. In the present study, it was demonstrated that the application weight and the moisture content can be predicted with errors (RMSEP) of 1.2 g/m² and 0.35 wt%, respectively [2]. However, it is obvious that cameras cover only widths in the order of one meter depending on optics and mounting height. The use of several cameras for a band width of e.g. 4 m is not a competitive solution from an economic point of view. Therefore, we tested the performance of a multiplex spectrometer system that was linked to 48 fiber-optic sensors mounted at intervals of 20 mm on a bridge spanning a conveyor with a width of 1 m (demonstration setup). Evidently, its spatial resolution is much lower than that of the camera (but still sufficient for process control), but the prediction errors for quantitative data were found to be only marginally

higher than those obtained with the camera: 1.4 g/m² for the application weight and 0.45 wt% for moisture [3].

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P03. HYPERSPECTRAL IMAGING DATA COMBINED WITH CLIMATE DATA TO PREDICT STOMATAL CONDUCTANCE AND TRANSPIRATION OF GRAPEVINE PLANTS

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Digital agriculture driven by new intelligent sensors is one of the main ways to improve farm management. Accessing physiological variables such as transpiration (E) and stomatal conductance (gs) in real time with optical instruments is challenging. These are the privileged variables to detect water stress. In this study, the objective is to evaluate visible-near-infrared spectral imaging data combined with climate data to predict transpiration (E) and stomatal conductance (gs) of grapevine (*Vitis vinifera* L.) plants by using Sequentially-Orthogonalized Partial-Least-Square Regression (SO-PLS).

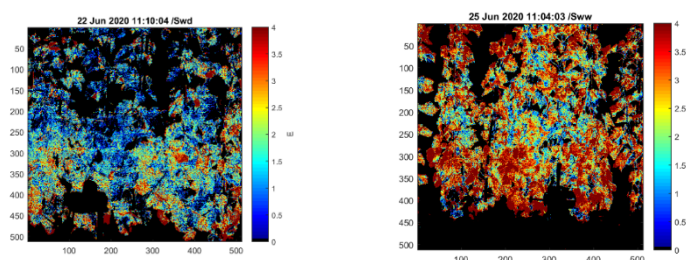


Fig. 1 Prediction of E on hyperspectral images of vines under (left) water deficit condition and (right) well watered condition.

A water stress gradient was obtained using pots of three grape varieties (Syrah, Merlot, Riesling) tested under two water conditions where precise monitoring of physiological variables was performed. Hyperspectral images were acquired and a weather station provided radiation (Rg), relative humidity (RH), temperature (Ta) and wind speed (Ws). For gs, best model is obtained by using only spectral data ($R^2= 0.656$, bias=8.76, RMSE=64.7 mmol.m².s-1). For E, the best model is obtained by using both blocks ($R^2= 0.699$, bias=0.055, RMSE=0.614 mmol.m².s-1). While E prediction model has a lower performance using only spectral data ($R^2= 0.625$, bias=-0.02, RMSE=0.67 mmol.m².s-1). These encouraging results offer prospects for the use of spectral imaging to detect water stress of grapevine plants.

P04. HYPERSPECTRAL IMAGING FOR MAPPING AND PREDICTION OF POLLUTANTS (ORGANIC AND TRACE ELEMENTS) IN SEDIMENT CORES

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Although trace elements (TEs) and hydrocarbons (HCs) contamination may occur naturally in sediments, anthropogenic inputs have become predominant in recent centuries. Sediments act as sinks for these pollutants, which are persistent and have high affinity for particulate matter. As a result, large amounts of them can accumulate in-depth and can alter nearby ecosystems and impact living organisms if sediments are mobilized. The best way to assess the risk induced by these pollutants is to sample and analyze sediment cores. However conventional analysis methods have the disadvantage of being time-consuming and requiring toxic extraction solvents. Recently, some researchers have investigated the application of coupling machine learning with visible and near-infrared spectroscopy for the determination of some contaminants in sediments and soils. Nevertheless, these studies generally focus only on surface measurements and are not suitable for sediment cores analysis due to the sample preparation process (sample denaturation). Hyperspectral imaging (HSI) is a promising tool for the contaminant analysis in sediment cores. This non-destructive technology has the advantages of significantly reducing analysis time and having a considerably higher spatial resolution (µm instead of cm). In this work, we propose a new

approach via a linear discriminant analysis (LDA) classification model to determine the chemical speciation of TE in sediments, the speciation playing a major role on their bioaccessibility. The LDA model (11 classes) created from hyperspectral images of spiked reconstructed sediments shows good overall predictions for the validation set in VNIR (visible and near infrared: 400-1000 nm) and SWIR (short wave infrared: 1000-2500 nm) domains, 0.74 and 0.83, respectively. Concerning organic pollutants (polycyclic aromatic hydrocarbons (PAHs) and aliphatic HCs), the influence of 6 factors on the pollutants hyperspectral response has been studied through experimental designs. As for TE, the same classification methodology was applied on PAHs and HCs, and showed good prediction accuracy. These promising results tend to confirm the feasibility of using HSI for high throughput analysis of organic and TE contaminants in sediment cores.

P05. CAPTURING HYPERSPECTRAL THERMAL IMAGES UTILIZING A FIRST ORDER SCANNING FABRY-PÉROT INTERFEROMETER

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Hyperspectral imaging in the thermal domain provide access to information, which is otherwise hidden when using passive, single-band thermography. This makes the technique suitable for various applications within different industries. In this presentation, a technical description of a novel hyperspectral thermal camera is provided, followed by *four* application examples. The camera system utilizes a first order scanning Fabry-Pérot interferometer (FPI) to capture data cubes of wavelengths ranging from 8 μm to 14 μm . The FPI functions as a variable bandpass filter where the separation distance between the mirrors determines the distribution of wavelengths which are transmitted to the sensor array.

1) Traditionally, when a thermal camera is used to determine the temperature of objects, it must be calibrated to the specific material, the object is made of. This usually limits the camera to measuring a single material at a time. Different materials (and surface finishes) possess different emissivities, which is a material specific, wavelength dependent parameter describing the amount of thermal radiation emitted by the object. We show a hyperspectral

thermal camera allows for simultaneous multimaterial temperature determinations as reported by A. Jørgensen et al [1]. Specifically, the study shows how a logistic regression model can be used to classify different dielectric substrates and subsequently determine their surface temperatures using a PLS model. The samples are heated to temperatures ranging from 27.1°C to 97.0°C and measurements of their surface temperature are evaluated to lie within 1.10°C of the true temperature.

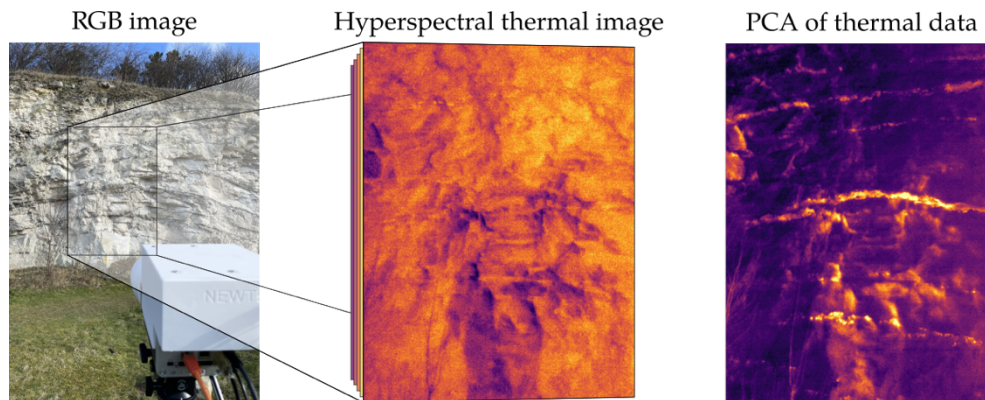


Fig. 1. Flint layers in limestone profile are clearly visible when using the hyperspectral information accessible in the thermal domain. The data is captured at Boesdal limestone quarry.

2) Apart from temperature measurements, the hyperspectral capability of the system enables it to detect and identify different organic gasses such as methane and ethylene from the molecular absorption bands. In this regard we demonstrate how the recorded FPI spectra can be correlated with corresponding FTIR spectra of the same gasses.

The camera has also been put to use in the field, where it has been used to 3) detect flint layers in a cliff face primarily consisting of limestone (Fig. 1) as well as 4) detecting underlying structural features in house walls.

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P06. COMBINATION OF MULTIVARIATE CURVE RESOLUTION WITH FACTORIAL DISCRIMINANT ANALYSIS FOR THE DETECTION OF FLAVESCENCE DORÉE GRAPEVINE DISEASE USING HYPERSPECTRAL IMAGING

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Hyperspectral imaging is an emergent technique in viticulture that can potentially detect bacterial diseases in a non-destructive manner. However, the main problem is to handle the substantial amount of information obtained from this type of data, for which reliable data analysis tools are necessary. The aim of this study is to offer a new efficient protocol based on hyperspectral imaging and data analysis tools to detect grapevine diseases.

The proposed data analysis workflow relies on two steps :

- a) Multivariate curve resolution-Alternating Least Squares (MCR-ALS) model [1] to provide chemically meaningful spectral signatures and related distribution maps of the image constituents. This unmixing method allows a global differentiation between infected and healthy images. However, some components related to the two different class types (infected and healthy pixels) may overlap, and hence, a supervised discrimination method is necessary to achieve a harder separation between them.
- b) Factorial discriminant analysis (FDA) model [2] on MCR scores (distribution maps). This supervised classifier will help to discriminate between infected and healthy images, using previous pixel labelling (classes infected or healthy). Such an approach is presumably more powerful than the direct use of FDA on the raw imaging data, since MCR scores are compressed and noise-filtered information on pixel properties, which makes them more suitable for discrimination analysis.

This combination of unmixing image and discrimination multivariate analysis method was tested on the case study of the Flavescence dorée. High levels of correct pixels discrimination rates (CR=85,1%) for the MCR-ALS/FDA discrimination model were obtained. The model present a lesser ability to determine infected leaves than healthy leaves. Nevertheless, only two images were misclassified. Therefore, proposed strategy constitutes a good approach

for the detection of the Flavescence dorée that could be potentially used to detect other phytopathologies.

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P07. EXCITATION-EMISSION HYPERSPECTRAL IMAGING AND CHEMOMETRICS FOR THE STUDY OF PLANT TISSUES

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Studying plant tissues is challenging due to the large variety of biological compounds present and the complexity of plant structures. Excitation-Emission Fluorescence Hyperspectral Imaging (EEM-HSI) is a powerful tool to study the rich variety of fluorophores presents in the vegetal tissues [1], since EEM-HSI provides a complete 2D Excitation-Emission fluorescence landscape per pixel, generating 4D images (with two spatial pixel dimensions and the excitation and emission directions) [1,2]. However, obtaining EEM-HSI requires a compromise between a sufficiently long acquisition time to obtain a good signal-to-noise ratio, but not too long to avoid the photobleaching effect, i.e., the degradation of the fluorescence signal of the fluorophores because of laser exposure. Thus, studying the photobleaching phenomenon is required to ensure a proper acquisition of EEM-HSIs. Added to the imaging photobleaching complexity, EEM-HSIs furnish massive data sets and chemometric tools are needed to interpret and extract the relevant information from the images.

In this work, EEM-HSIs images have been used to characterize the constituents of *Oryza Sativa* root rice cross-sections. To obtain optimal results, the photobleaching phenomenon was studied first by acquiring consecutive fluorescence images on the same sample at different times. Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) [3]

was used to analyze the photobleaching data and extract the information linked to the pure fluorophores present in the sample, expressed by their distribution maps, fluorescence profiles and degradation curves. The results of this photobleaching study indicated a significant and distinct degradation in several fluorophores and drove the conditions to perform future EEM-HSI for plant tissue characterization. Thus, EEM-HSI acquisition for root cross-section characterization was carried out reducing the full range of excitation wavelengths to work only with the most representative excitation channels, achieving a good signal-to-noise ratio, a very low photobleaching effect and a significant reduction of the image size to be analyzed. MCR-ALS was used to study these optimized EEM-HSI and provided reliable distribution maps and excitation-emission landscapes for the fluorophores present in the plant tissues.

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P08. HYPERSPECTRAL IMAGING AND A DEEP NEURAL NETWORK FOR DETECTION OF DAMAGES IN ‘ROJO BRILLANTE’ PERSIMMON

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‘Rojo Brillante’ persimmon is a fruit with high social and economic importance in the Valencian region of Spain. It is a delicate product, which can easily suffer damages during harvest and post-harvest handling. Mechanical damage is the main cause of flesh browning in this fruit, and an early detection will avoid the damaged product to arrive to the consumer. It is usually undetected during the post-harvest inspection whereas it is when the consumer peels it.

130 persimmons were used in the experiment. They were artificially damaged with a controlled force, and hyperspectral images (450-1050 nm) of each persimmon were taken before and after being damaged. After the damage, they were measured every day for three days, obtaining a total of 650 images. Since the damaged area was known, the spectral reflectance of the damaged and undamaged areas in the persimmon were split into two individual databases to train and validate the Deep Neural Network (DNN). The DNN was built using 12 fully connected layers, which processed 60 spectral bands and two predictive classes (healthy and damaged classes). Results showed that the DNN model successfully detected the labelled bruise with a 99% Recall. Compared to the results previously obtained in a previous study [1], the DNN model detected damaged regions located on the surrounding border of the labelled bruised, which were “invisible” to their previously used supervised algorithm and are, in fact more realistic. Thus, that indicates the high accuracy of the neural network.

The results showed that neural networks (the used DNN) together with hyperspectral imaging techniques have great potential to detect invisible damage regions in fruit and, therefore, can be used to detect mechanical damages in persimmon sorting lines.

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P09. SEMANTIC SEGMENTATION OF ROOF MATERIALS IN URBAN ENVIRONMENT BY UTILIZING HYPERSPECTRAL AND LIDAR DATA

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Mapping areas in an urban environment can be challenging due to the variety of materials and manmade structures. Urban environment is a mix of natural and artificial materials, and to find the right object with a specific material is a challenge even for the trained eye. Therefore, by applying hyperspectral (HS) imagery it is possible to examine surface materials based on their spectral signature, and LiDAR for detecting the geometrical structure of an object. These data can be exposed to a machine learning algorithm to automatically recognize objects, and in this study buildings and roof materials are investigated.

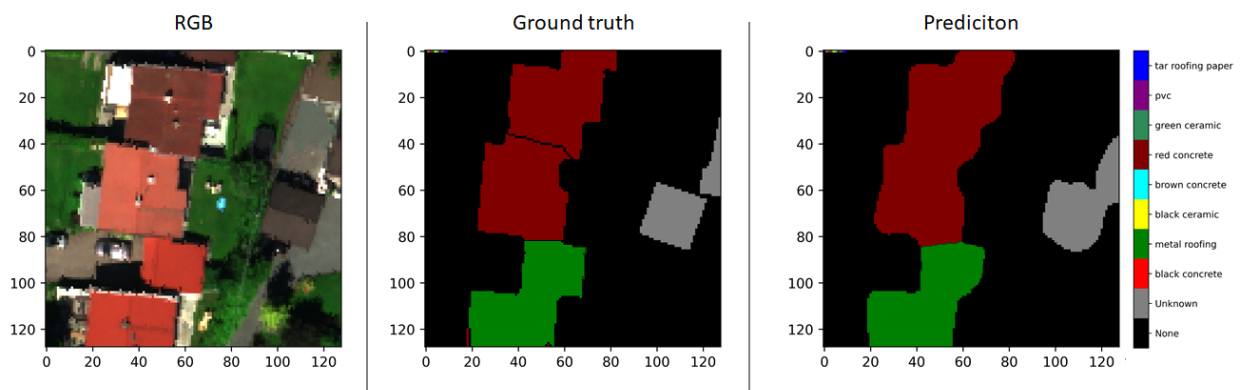


Figure 1: Model prediction of roof materials in the urban environment.

This study presents an application of semantic segmentation for roof materials based on fused HS (HySpex VNIR-1800 and SWIR-384) and LiDAR (Riegl VQ-560i) data acquired from 2021 over Bærum municipality near Oslo in Norway. By using a U-net and Resnet34 architecture approach on airborne images, it is possible to localize and classify roofs in urban environments, as depicted in Fig.1. The ground truth is generated using information from field work, a geographical database for buildings and the watershed algorithm for object detection. The HS and LiDAR data have almost 400 spectral and spatial features a supervised neural network deems and learns. The network then returns a prediction mask of the roofs' positions and materials. Analysis like this has a great potential to automate several mapping chores and manual assignments.

P10. SHADOW DETECTION AND SEMANTIC SEGMENTATION USING HYPERSENSPECTRAL IMAGING, LIDAR AND MACHINE LEARNING

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Urban regions consist of different types of vegetation, complex materials, and structure information, which can be collected by remote sensing. One of the biggest problems within remote sensed data is the appearance of shadows, as it may lead to confusion and misleading results. Shadow detection is required to increase the performance level of the image segmentation and to distinguish between for example roads and non-roads, asphalt and shadow on asphalt. Shadow detection based on deep learning algorithms can reduce the impacts of the errors and produce a better result.

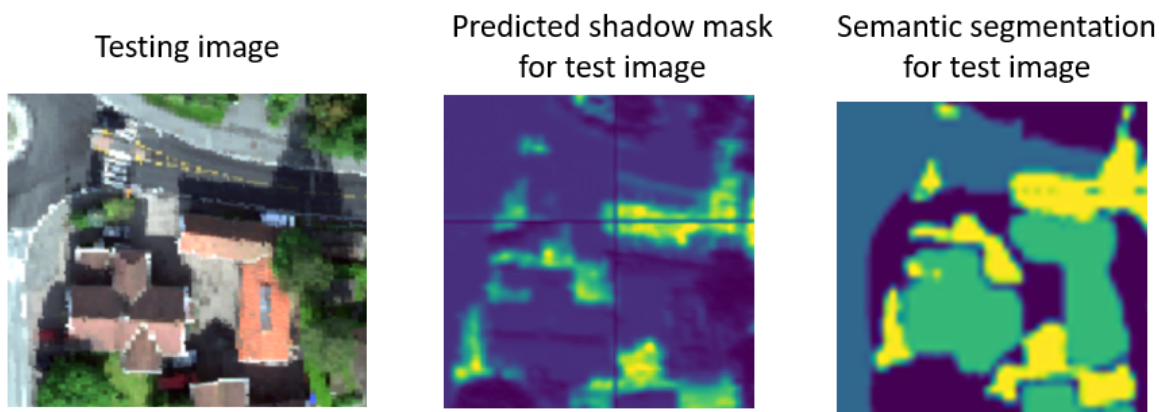


Figure 2: Prediction of shadow mask and semantic segmentation on a test image

In 2019, hyperspectral (HS) and LiDAR data from urban areas in Bærum municipality in Norway was acquired. In this study, shadow detection and semantic segmentation were carried out based on the fused HS (Hypex VNIR-1800 and SWIR-384) and LiDAR (Riegl VQ-1560i). In order to detect shadow, a shadow mask produced from SWIR and LiDAR was used to train a U-net model. The model was successfully used to predict shadow mask for higher resolution images such as VNIR. With the generated shadow mask, shadow was identified as a class for semantic segmentation with a U-net architecture (Figure 1). The classification accuracy was increased by introducing shadow classes.

P11. COMBINATION OF RAMAN MICROSCOPY AND SCANNING ELECTRON MICROSCOPY TO UNDERSTAND LODGING RESISTANCE IN TEF

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Tef (*Eragrostis tef*) is the most important staple crop in Ethiopia and Eritrea. Moreover, its grains are gluten-free and protein rich, so it is considered as a “super-food”. Adapting tef to modern farm practices is challenging due to its high lodging susceptibility that can cause a crop loss up to 50 %. Lodging describes the displacement of roots (root lodging) or fractures in the culm (stem lodging) forcing the plant to bend or fall from its vertical position. In tef, it is more likely that root lodging causes the damage [1]. In general, lodging is facilitated by various abiotic and biotic factors, e.g., wind damage and often occurs in overpopulated fields.

We aim to understand the structural and chemical properties underlining tef susceptibility / resistance to lodging on a structural-microscopic level. Tef genotypes of showing either resistance or susceptibility to lodging in field experiments[2] are subjected to histological characterization acquired by light and scanning electron microscopy (SEM), and microchemical analyses obtained by Raman microscopy and Energy-dispersive X-ray spectroscopy (EDX). Cross-sections of roots and internodes, were compared between genotypes of contrasting tendency to lodge. Our preliminary experiments have shown an early development of tissue voids as aerenchyma or hollow stem, and intensive lignification in the lodging-prone, as compared to lodging-resistant genotype. Combination of Raman maps and elemental and topographical SEM-EDX maps, as well as additional phenotypical information in a variety of thoroughly characterized tef genotypes will shed light on tef lodging and towards prevention or reduction of lodging in the field.

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P12. HYPERSPECTRAL IMAGING TO DISCRIMINATE THE COLORS OF POMPEII AND CINNABAR PIGMENT DEGRADATION PRODUCTS

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The palette of pigments used by Roman artisans to create the wall paintings of Pompeii, Italy, was composed mainly by earth pigments and more expensive pigments such as Egyptian blue or red cinnabar, among others. To avoid/reduce sampling process in their study once included in wall paintings, non-invasive and portable instrumentation becomes essential.

In this work, hyperspectral imaging in the SWIR range (HySpex SWIR-640 camera, 960-2500 nm) has been used to discriminate the nature of some specific pigments from the Pompeian pigment palette. For that, a spectral library has been created from reference pigments already known to be present in the Pompeian wall paintings. Then, these samples have been analyzed in the laboratory, as a preliminary step to the in-situ strategy, and a combination of K-means clustering and correlation algorithms have been used [1]. Moreover, cinnabar decorated fresco mock-ups have been subjected to accelerated weathering in order to mimic the blackening of this pigment. The results obtained using multivariate curve resolution (MCR) [2] allowed to discriminate for the first time cinnabar (α -HgS) from calomel (Hg_2Cl_2), this last, one of the main deterioration products usually monitored in situ through Raman spectroscopy [3]. These preliminary results could pave the way to construct, in the future, a methodology for a semi-quantitative assessment and mapping of transformation products of pigments on mural paintings.

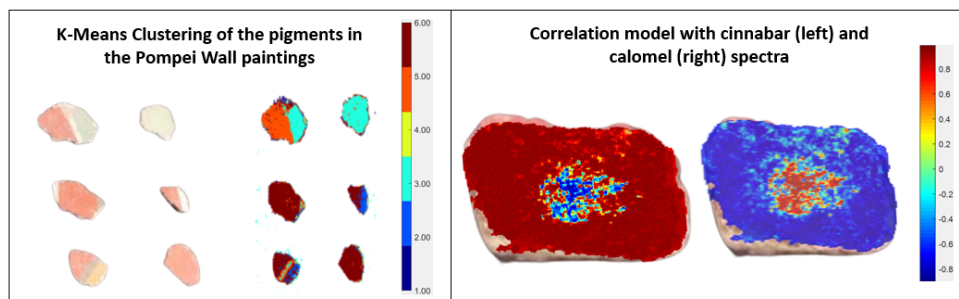


Fig. 1. Results of the discrimination of pigments in the Pompeian walls (left) and differentiation of cinnabar vs calomel (right).

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P13. COUNTERFEIT DETECTION IN TURMERIC POWDER SAMPLES BY USING HYPERSPECTRAL RAMAN SPECTROSCOPY

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Phytotherapy, can be defined as, 'treatment with plants or plant components'. Nowadays, because of these products are made by plants, they are considered as more 'natural' than pharmaceutical drugs. Sometimes these phytotherapy products do not have the same fast and direct effect in the human being than pharmaceutical drugs, and this make these phytoproducts less competitive against pharmaceutical drugs. For this reason, some natural products are doped with active pharmaceutical ingredients in order to give to this 'natural product' the same effect of pharmaceutical drugs getting the marketing goal of being a 'natural product' which produces the belief to the costumer of being taking a healthier product.

In this study turmeric powder samples have been analyzed by a Raman Hyperspectral instrument for detecting counterfeit samples. Curcumin can be found in turmeric powder between the range of 7-13%, in this study the curcumin will be quantified and by this way counterfeit samples can be detected. For the curcumin quantitation in turmeric powder

samples, the purposed method to analyze these samples is Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS), a method without any previous calibration model [1]. MCR-ALS allowed obtaining concentration maps for curcumin and therefore, consequent analysis of the curcumin distribution in the turmeric powder samples.

Results certified the ability of this method for quantifying and also for detecting counterfeit samples of turmeric powder. As a matter of fact, the quality of the results demonstrated the useful of encompassing Raman Imaging techniques with MCR-ALS and, consequently, the assessment of the turmeric powder effect's authenticity.

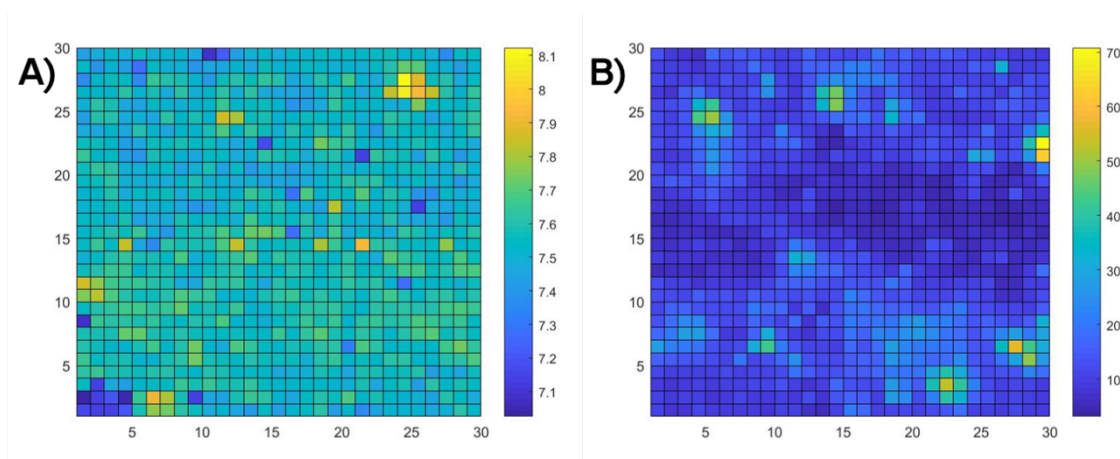


Fig. 1. Curcumin concentration maps in: A) real turmeric powder sample B) curcumin doped turmeric sample

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P14. COMPARISON OF MSC AND EMSC IN THE SPECTRAL ANALYSIS OF SCOTS PINE SAPWOOD AFFECTED BY DECAY FUNGI

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In this study, a short-wave infrared (SWIR) hyperspectral camera was used to analyze different degradation stages of Scots pine sapwood (*Pinus sylvestris* L.) specimens inoculated with monocultures of either a brown rot fungus (*Rhodonia placenta* Fr.) or a white rot fungus (*Trametes versicolor* L.).

Data analysis was performed using Partial Least Squares (PLS) algorithm with the mass loss due to fungal decay as the response variable. This study shows that the images of a SWIR hyperspectral camera are suitable for predicting wood mass loss due to basidiomycete decay, and suitable for the characterization of the type of fungal decay.

Two pre-processing methods are compared in this presentation: the simple Multiplicative Signal Correction (MSC) and the more advanced Extended Multiplicative Signal Correction (EMSC). The MSC estimates an offset and a scaling for each of the spectra [1], while EMSC extends this two-parameter model by adding two wavelength dependent parameters and any known spectra. [2,3]

Library spectra of the main wood polymers cellulose and lignin are used in the data analysis for both analysis approaches. For MSC pre-processing, the spectra of cellulose and lignin are used to explain the PLS loadings and correlation coefficients. For EMSC pre-processing, the relative amounts of cellulose, and lignin are estimated, in addition to more advanced (wavelength dependent) scattering characteristics. This provides additional insights in the changes that occur in the wood during the decay process, but it does not necessarily improve the prediction of the mass loss, which is the common response variable in the measurement of fungal decay.

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P15. HYPERSPECTRAL IMAGING APPLIED TO MATERIAL CHARACTERIZATION OF BRICK BUILDING FACADES

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The manufacturing of clay bricks comprising brick building facades represents a substantial carbon footprint, in addition to its financial cost. As such, there is great value in both the preservation and recycling of brick building facades. Monitoring the degradation of such

facades, both to evaluate possible preventive measures and to contribute to brick recycling, is therefore worthy of scientific research. This study suggests the use of hyperspectral (HS) imaging as a means for material characterization of brick building facades in situ.

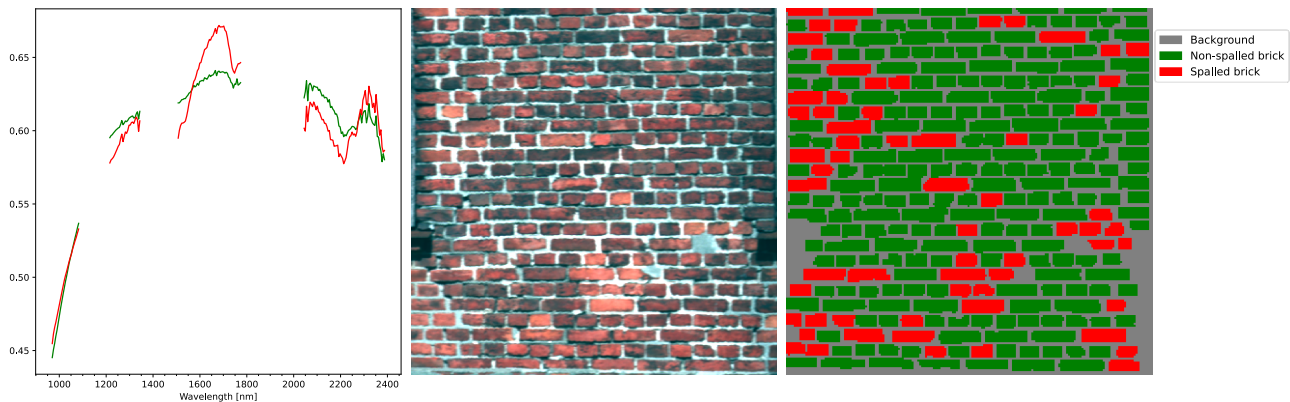


Fig. 1. Left: EMSC corrected mean SWIR spectra of labelled bricks. Middle: RGB VNIR bands of sub-image. Right: PLSDA predictions using SWIR data of segmented bricks.

The case site for this study is the brick building “St. Olavs Vold” in Sarpsborg, Norway. The building in question was constructed in the mid-19th century and is in an advanced state of degradation. HS images in the VNIR and SWIR spectral ranges were recorded using a Hypspx Mjølner VS-620, mounted on a rotation stage. Limited ground truth data is known at the early stage of this study, but certain brick qualities, such as brick spalling, are observable from the field. Preliminary results show that damage such as spalling can be detected both in the VNIR and SWIR ranges using PLS-DA, see Fig. 1. The classifier shown in Fig. 1 was trained on the EMSC-corrected average spectra (SWIR) of labelled bricks. The model was validated using k-fold cross-validation and shown to have an average test accuracy of 89.4%. Though initial results for detecting existing damages are promising, the objective of this study is to ascertain which brick characteristics may give early warning of future damages, before they occur.

P16. CLASSIFICATION OF FOUR FUNGAL PLANT PATHOGENS BASED ON CULTURE AGE USING HYPERSPECTRAL IMAGING

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The wide consumption of maize in South Africa has made the study of fungal pathogens associated with this staple crop a high priority. Crop diseases such as Gibberella Ear Rot (GER), Fusarium Ear Rot (FER) and Diplodia Ear Rot (DER) caused by *Fusarium* spp. and *Stenocarpella* spp. are hindrances to ensuring food security for populations who depend on this vital source of nutrients. Of additional concern, certain pathogens, such as *Fusarium* spp. pose a risk to food safety through the production of mycotoxins. Previous studies have been able to distinguish between different fungal pathogens [1], [2] However, the effect of colony age has not been widely studied. Moreover, only three species have been compared at once.

Four species of fungal pathogens, namely *F. verticillioides* (MRC826), *F. graminearum* (M14-55), *F. boothii* (M0100) and *Stenocarpella maydis* (SM8) were inoculated in triplicate on potato dextrose agar (PDA). Each species was incubated for 3, 5 and 7 days at 25°C, respectively. Hyperspectral images were acquired using a SisuChema SWIR (920-2514 nm) pushbroom imaging system. Data analysis was conducted mainly using Python v. 3.8.8. Extraction of the region of interest and segmentation was conducted using the workflow described in Figure 1.

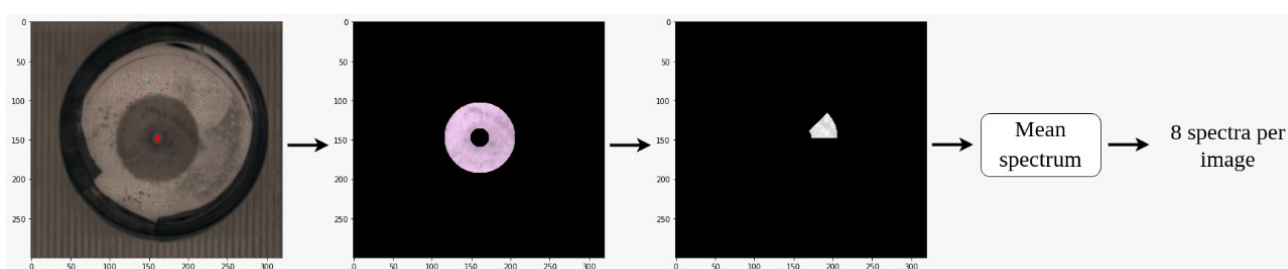


Fig. 1. Extraction and segmentation of region of interest from raw image for object-wise analysis

Various classification algorithms were assessed with the best classification accuracy being achieved on Day 3 (100%), after which classification accuracy decreased over time. This study suggests that spectral variables related to species classification are more prominent in younger fungal cultures.

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P17. CONTROL OF THE POLYTETRAFLUOROETHYLENE (PTFE) COATING BY RAMAN MAPPING

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In the coatings industry it is common to incorporate particles into the deposition metal matrix in order to improve properties of the material. The polytetrafluoroethylene (PTFE) is one of the most widely used particles in Ni-P electroless processes because of, among other properties, the high corrosion resistance and lower friction of the resulting Ni-P/PTFE coatings [1]. However, these properties are highly dependent on the composition of the deposit, which must be homogeneous all over the surface, therefore, quality control of the coating level is very important.

One of the simplest way to carry out a non-destructive control of the coated plates is visual inspection, both manual and by using analysis of digital images [2]. However, despite the sensitivity of such methods is good enough to distinguish between coated and non-coated parts, it is not acceptable when it comes to evaluate the composition of Ni-P/PTFE coatings. In this case, spectroscopic methods, in particular Raman spectroscopy, can be beneficial as PTFE has several characteristic Raman bands [3].

In this work Raman spectroscopy has been applied for qualitative analysis of the homogeneity of the PTFE coating on metal plates. A characteristic peak at 734 cm⁻¹ has been identified in Ni-P/PTFE coating and used for the control of the coating level. The experiments have shown that the peak is detectable, even for the samples with low thickness of the coating, by using longer exposure time. In order to evaluate spatial distribution of the coating level, the spectra were taken using 10 x 4 grid of sampling points uniformly distributed over the surfaces, which made possible to construct distribution maps.

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P18. COMPARISON OF DIFFERENT ILLUMINATION SYSTEMS FOR MOISTURE PREDICTION IN CEREAL BARS USING HYPERSPECTRAL IMAGING TECHNOLOGY

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Moisture content and distribution is a critical parameter in bars production. A wrong control of moisture can lead to non-conforming products and waste excess on production lines. In the field of hyperspectral imaging, the search for alternative light sources to stabilized-halogen (cheaper and emitting less heat) is a growing necessity for the application of this technology in industry.

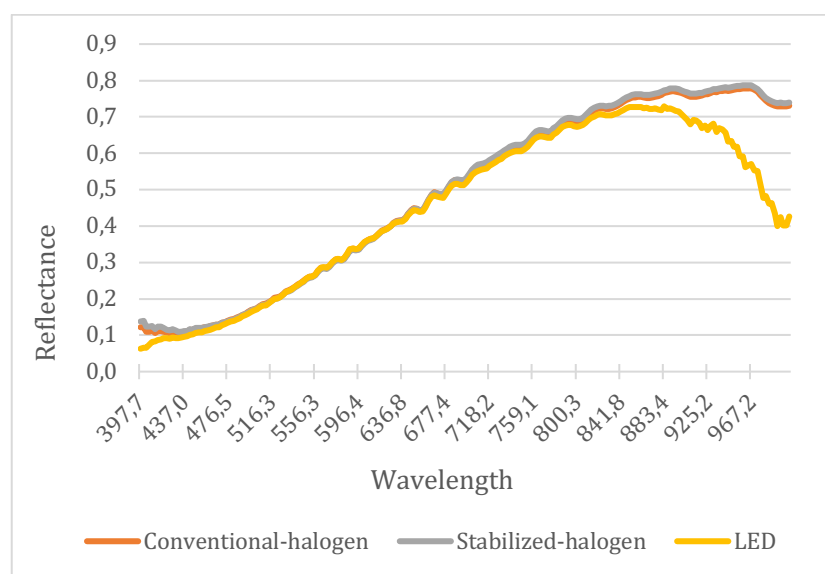


Fig. 1. Spectra comparison between halogen-based and LED-based systems.

This study presented the comparison between three different illumination systems for the moisture prediction in the VIS-NIR range (from 400–1000 nm). The hyperspectral images were acquired using three illumination systems including two halogen-based systems (stabilized-halogen and conventional-halogen) and a LED-based illumination system.

The results showed that halogen-based illumination systems combined with a PLS model performed better prediction of humidity in cereal bars. Lower accuracies were obtained when performing the experiment with LED-based illumination system, showing double the error obtained in both halogen-based systems. It was concluded that this is a consequence of the data that is lost in bands appearing after 850 nm that may be revealing information about the moisture in bars since the second overtone of water O-H is found at 970 nm. The results demonstrated that conventional halogen-based light systems in the VIS-NIR range are promisingly useful for humidity prediction in cereal bars.

P19. BAYESIAN OPTIMIZATION FOR CHANNEL SELECTION FOR MULTISPECTRAL IMAGING IN PLANT STATUS MONITORING

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Spectral imaging is a widely employed tool in plant phenotyping and plant disease identification [1]. While hyperspectral imaging provides fine-granular spectral features, the limited availability of labeled data for plant disease identification does often not satisfy the large number of parameters to be trained in the high-dimensional hyperspectral space. Multispectral cameras with only a few spectral channels do not provide the same amount of spectral detail, but are typically more affordable, easier to handle and computationally more efficient. Existing state-of-the-art image processing algorithms can be extended with additional channels to process multispectral images and explicitly consider the spatial pattern or area covered by disease symptoms. Several wavelength selection algorithms have been proposed in the literature with the aim to lower the computational burden of hyperspectral images. However, they are typically not suitable for selecting channels for multispectral cameras since they focus on single spectral features that cannot be easily translated into broadband filters of multispectral cameras. We propose an approach for the

configuration of problem-specific multispectral channels based on Bayesian Optimization from hyperspectral information. Our approach considers the applicable constraints of optical systems such as feasible filter functions and filter width. We expect that our formalism can contribute to a more widespread and more efficient use of spectral imaging for disease identification in the future.

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P20. STUDY OF THE COMBINATION OF COLOR (RGB) AND NIR HYPERSPECTRAL IMAGES TO IMPROVE UNMIXING USING MULTIVARIATE CURVE RESOLUTION

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Hyperspectral images (HSI) are chemical pictures that provide spatial and chemical information about samples [1]. This spatial information is important in some applications such as the assessment of heterogeneity during the blending of food or pharmaceutical products as well as the morphology and composition of biological tissues. On the other hand, accessible yet effective color images based on the RGB (Red, Green and Blue) space coordinates can be obtained from samples using simple imaging systems such as smartphones or webcams. RGB-based color images satisfactorily define, in many cases, different regions of the sample; instead, to provide well-defined chemical information, NIR measurements are required. The information provided by RGB images can be potentially used as complementary information to improve the unmixing performance of chemometric tools such as Multivariate Curve Resolution (MCR), giving solutions that are more accurate and a comprehensive vision of the sample.

In this work, a dual sensor system was designed coupling an RGB webcam to a near-infrared hyperspectral imaging (NIR-HSI) pushbroom system. The system was used to obtain images using both sensors from samples consisting of cellulose substrates and polymeric plastic films with different color pigments and composition. Correction of image distortion and alignment between the images obtained by the two sensors was required. Additionally,

spectral preprocessing of the NIR-HSI data and RGB images was carried out. Afterwards, the combined image data was analyzed with MCR to solve the mixture analysis problem through a bilinear model to generate pure distribution maps and related spectral fingerprints of the components in the image [2]. The results obtained have shown that the RGB and NIR-HSI image fusion provides more accurate distribution maps and combined NIR/RGB fingerprints for the components in the systems studied.

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P21. USING 3D CONFOCAL RAMAN IMAGE AND MIXTURE DESIGN OF EXPERIMENTS DURING PREFORMULATION DEVELOPMENT TO DETERMINE LOCAL AND GLOBAL MISCIBILITY OF EXCIPIENTS

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Excipient's homogeneity is of paramount importance during the development of appropriate pharmaceutical formulations due to its relation to stability, safety and efficacy. Raman imaging offers a direct, unique and easy way to this evaluation since different compositions between surface and core of preformulation samples followed by 3D Raman imaging allow determining phase separation in the very early stages of development. Here confocal Raman microscopy was used to evaluate the miscibility between Apifil®, Capryol® and Transcutol® with butamben, a local anesthetic. Homogeneity was determined throughout nanostructured lipid carriers preformulations, and the best proportions between the local anesthetic butamben and solid and lipid excipients was obtained. Mixture experimental design (DoE) was employed to better evaluate the variation of the excipients concentration, allowing us to conclude that Transcutol® worsen the miscibility while Capryol® enhances this parameter. However, the excess of liquid lipid leads to phase separation, a feature

clearly highlighted by Raman 3D images. Two ratio proportions between the excipients were found as good miscibility: Solution 1: Apifil® 30.00% (w/w), Capryol 20.00% (w/w) and Transcutol 10.00% (w/w), with desirability of 0.783; and Solution 2: Apifil® 25.00% (w/w), Capryol 25.00% (w/w) and Transcutol 10.00% (w/w), with desirability of 0.742. These results highlight a new vision to pharmaceutical formulation development.

Acknowledgment

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P22. RAMAN IMAGING OF VATERITE INCLUSIONS IN FISH OTOLITHS

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Within the inner ear of bony fishes is a calcareous structure called an otolith, usually consisting of aragonite (a polymorph of calcium carbonate).¹ The presence of vaterite (an abnormal polymorph) in fish otoliths has been shown to cause hearing impairment in fish and can be detrimental to their survival.² It has been hypothesised that changes in this calcium carbonate structure also influence the fish's navigation skills. Using Raman imaging we have detected the presence of vaterite in fish otoliths found in New Zealand waters.

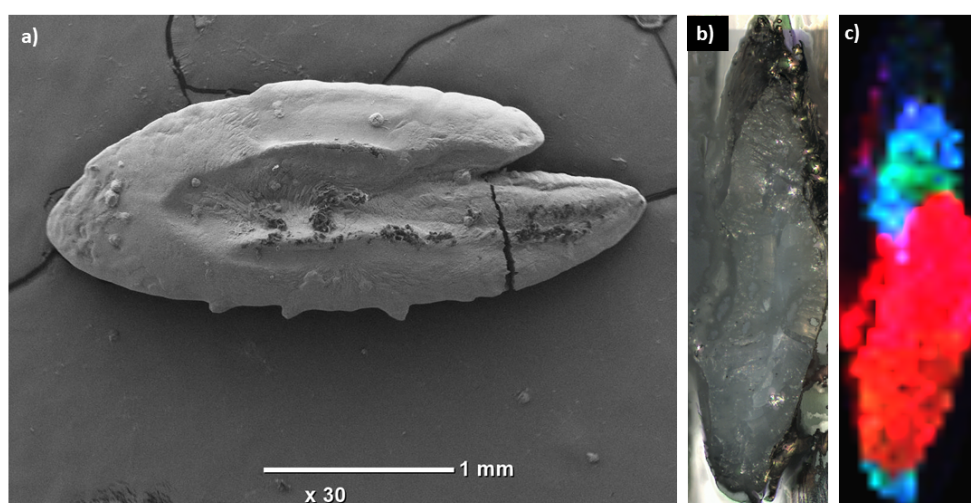


Fig. 1. a) SEM image of fish otolith face. b) Microscope image of fish otolith inside edge. c) Raman image showing presence of aragonite (red) and vaterite (blue and green).

A Horiba confocal Raman microscope was used to map the calcium carbonate polymorph on the surface of several fish otoliths and found that some indicate zones of vaterite inclusions (see Fig.1). These vaterite containing otoliths can potentially be linked to fish that have been found far from their normal habitat, and hence correlated with navigational problems.

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P23. RECONSTRUCTION OF HYPERSPECTRAL CUBES FROM CTIS IMAGES – COMPARISON AMONG THE EM ALGORITHM, CNNs AND A HYBRID APPROACH

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The Computed Tomography Imaging Spectrometer (CTIS) is a simple, compact and affordable snapshot Hyperspectral Imaging (HSI) system. It creates a 2-D image by the diffractive optical element that diffracts a 3-D hyperspectral cube into the zeroth and surrounding first orders as shown in Fig. 1. The reconstruction of hyperspectral cubes from CTIS images entails broad applications of the CTIS technique.

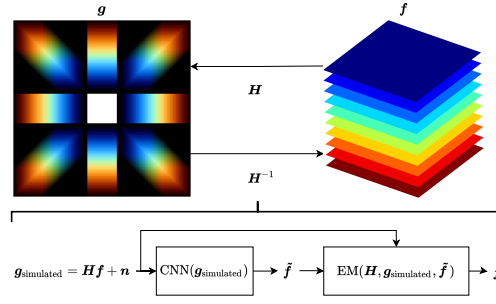


Fig. 1. Top: The connection between a CTIS image and a hyperspectral cube. Bottom: The hybrid approach workflow.

We applied Convolutional Neural Networks (CNNs) to the hyperspectral cube reconstruction [1] that are faster, more accurate and less susceptible to image noise than the traditional Expectation Maximization (EM) algorithm. An important caveat is that the CNNs must see data of different geometries to generalize well to images of new objects. To follow up, we propose a hybrid approach [2] which sequentially combines a CNN and the EM algorithm. The hybrid approach achieves a better performance than the EM and CNN alone and can manage new data to which the CNN is not exposed during the training phase.

The work is based on the collaboration between Newtec Engineering A/S and University of Southern Denmark.

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