International Association
for Spectral Imaging

IASIM - 2012
September 9-14, 2012
Sigulda & Jurmala, Latvia

IASIM Scientific Conference, September 12 – 14, 2012

This IASIM meeting will include two full days of scientific sessions covering all aspects of spectral imaging. Oral and poster presentations are invited on any facet of spectral imaging research. A partial list of possible topics includes:

- Imaging instrumentation
- Spatial / Spectral analysis algorithms
- Feature identification or quantification
- Real-time image processing
- Data compression and transformation
- Multispectral / Hyperspectral applications

Technical sessions will include presentations by invited speakers & opponents, short individual presentations, and panel discussions from members of the imaging community.

This two day scientific conference will be held in the Latvian beach resort area of Jurmala at the Baltic Beach Hotel www.balticbeach.lv/en.

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IASIM-12 Hyperfest Workshop - Hotel Ezeri Spa, Sigulda, Latvia

Sunday, 9 September

16:00 Bus pickup at Riga International Airport

16:30 Alternate bus pickup near Old Riga

19:00 Dinner / socializing

Monday, 10 September

08:00 – 09:00	Registration
09:00 – 12:30	Opening comments / Session I
10:30 – 10:45	Coffee break
12:30 – 13:30	Lunch
13:30 – 17:00	Session II
15:00 – 15:15	Coffee break
17:00 – 18:00	Problem solving session
19:00 – 20:00	Dinner

Tuesday, 11 September

09:00 – 12:30	Session III
10:30 – 10:45	Coffee break
12:30 – 13:30	Lunch
13:30 – 20:00	Latvian Culture & History Excursion
20:00 – 21:00	Additional problem solving session (optional)

Wednesday, 12 September

09:00 – 12:00	Session IV
10:30 – 10:45	Coffee break
12:00 – 13:00	Lunch
13:00 – 16:00	Session V
16:15 – 18:00	Transportation to IASIM Conference, Jermala

IASIM-12 Scientific Conference – Baltic Beach Hotel Spa, Jurmala, Latvia

Wednesday, 12 September

18:00 – 21:00	Registration
19:00 – 22:00	Social Reception

Thursday, 13 September

08:00 – 09:00	Registration
09:00 – 12:30	Opening comments / Session I
10:30 – 10:45	Coffee break
12:30 – 13:30	Lunch
13:30 – 17:00	Session II
15:00 – 15:15	Coffee break
18:00 – 19:00	Social Reception
19:00 – 23:00	Conference Dinner

Friday, 14 September

09:00 – 12:30	Session III
10:30 – 10:45	Coffee break
12:30 – 13:30	Lunch
13:30 – 17:00	Session IV
15:00 – 15:15	Coffee break

ABSTRACT LIST

Surname	Name	Title	Type of Presentation	Page
Geladi	Paul	THE IMPORTANCE OF BEING LOCAL: HYPERSPECTRAL NEAR-INFRARED IMAGING APPLICATIONS IN WOOD TECHNOLOGY FOR BIOMASS AND BUILDING MATERIALS.	oral	6
Tena Pajuelo	Noelia	AUTHENTICITY OF DDGS - BOTANICAL ORIGIN CLASSIFICATION BY NEAR INFRARED MICROSCOPY	poster	7
Williams	Paul J	NEAR-INFRARED HYPERSPECTRAL IMAGING AND MULTIVARIATE IMAGE ANALYSIS TO CHARACTERISE FUSARIUM SPECIES ON GROWTH MEDIA	oral	8
Carstensen	Jens M	BISCUIT CHEMICAL MAPPING - MOISTURE AND BROWNING	oral	9
Ahlinder	Linnea	IN VITRO STUDY OF UPTAKE AND INTERNALIZATION OF OXIDE NANOPARTICLES IN THE CELL NUCLEUS BY RAMAN MICROSPECTROSCOPY AND MULTIVARIATE DATA ANALYSIS	poster	10
Edelman	Gerda	HYPERSPECTRAL IMAGING FOR THE IDENTIFICATION AND AGE ESTIMATION OF BLOOD STAINS AT THE CRIME SCENE	oral	11
Serranti	Silvia	NIR HYPERSPECTRAL IMAGING APPLIED TO CLASSIFICATION OF OAT AND GROAT KERNELS	oral	12
Carstensen	Jens M	NORMALIZED CDA FOR FAT/MUSCLE SEGMENTATION IN SALAMI	oral	13
Pirro	Valentina	INTERACTIVE HYPERSPECTRAL APPROACH FOR EXPLORING AND INTERPRETING DESI-MS IMAGES OF CANCEROUS AND NORMAL TISSUE SECTIONS	oral	14
Dinuls	Romans	IDENTIFICATION OF TREE SPECIES IN MULTISPECTRAL IMAGES	oral	15
Gulbe	Linda	IDENTIFICATION OF FOREST AREAS AND FOREST INVENTORY PARAMETERS IN MULTISPECTRAL SATELLITE IMAGES USING SUPERVISED CLASSIFICATION METHODS	oral	16
Møller	Flemming	QUANTIFICATION SALAMI COLOUR AND TEXTURE CHANGES	oral	17
Hans	Guillaume	MONITORING OF MOISTURE CONTENT AND BASIC SPECIFIC GRAVITY IN BLACK SPRUCE LOGS USING A HANDHELD MEMS-BASED NEAR-INFRARED SPECTROMETER.	poster	18
Ferrari	Carlotta	USE OF HYPERSPECTROGRAMS FOR DATA COMPRESSION AND INFORMATION EXTRACTION FROM HYPERSPECTRAL IMAGES	poster	19
Jakovels	Dainis	SKIN HEMOGLOBIN ASSESSMENT BY SPECTRAL IMAGING IN VISIBLE RANGE	oral	20
Xin	Zhang	MULTIVARIATE CURVE RESOLUTION AND ROTATION EVALUATION ON REMOTE SENSING HYPERSPECTRAL IMAGES	poster	21
Manley	Marena	EVALUATION OF CHEMICAL CHANGES IN NIR HYPERSPECTRAL IMAGES OF CEREALS USING CLASSIFICATION GRADIENTS	oral	22
Erkinbaev	Chyngyz	HYPERSPECTRAL SCATTER IMAGING FOR APPLE QUALITY EVALUATION DURING SHELF-LIFE STORAGE	oral	23
Diebele	Ilze	FOUR SPECTRAL BAND VIDEO-IMAGING DEVICE FOR SKIN DIAGNOSTICS	poster	24
Oliveri	Paolo	XRF HYPERSPECTRAL MAPPING OF PAINTED SURFACES FOR PAINTING CHARACTERISATION – A MULTIVARIATE EXPLORATORY APPROACH	poster	25
Lanteri	Silvia	A PCA-BASED HYPERSPECTRAL APPROACH TO DETECT EDIBLE MUSHROOMS INFECTED BY MYCOPHILIC FUNGI	poster	26
Sullivan	Carl	FEASIBILITY OF HYPERSPECTRAL IMAGING FOR PHARMACEUTICAL CLEANING VERIFICATION	oral	27
Patteti	Suman Babu	SPECTRAL CHARACTERISTICS OF IRON ORE MINERALS USING MODIFIED GAUSSIAN MODEL	oral	28
Valerijs	Garancis	DEVELOPMENT OF MULTISPECTRAL BIO-MEDICAL IMAGING SYSTEM	poster	29
Prats-Montalbán	José Manuel	OPTIMIZED EXTRACTION OF THE ARTERIAL INPUT FUNCTION IN PROSTATE DCE-MR IMAGES BY MULTIVARIATE IMAGE ANALYSIS	oral	30
Haddadi Goyaghaj	Ataollah	USE OF NEAR-INFRARED HYPERSPECTRAL IMAGES FOR LOG MOISTURE CONTENT DISTRIBUTION MAPPING	oral	31
Jung	András	NON-SCANNING HYPERSPECTRAL FRAME CAMERA FOR INDOOR AND OUTDOOR SPECTRAL IMAGING	oral	32
Piqueras Solsona	Sara	HYPERSPECTRAL IMAGE ANALYSIS BY ULTRAFAST RAMAN IMAGING.	poster	33
De Juan	Anna	IMAGE MULTISET ANALYSIS: ENHANCING IMAGE INFORMATION	oral	34
Gowen	Aoife A	DEVELOPMENT OF A SYSTEM FOR RAPID SCREENING OF WATER SAMPLES USING NIR CHEMICAL IMAGING	poster	35
De Juan	Anna	MULTIVARIATE CURVE RESOLUTION AND ROTATION EVALUATION ON REMOTE SENSING HYPERSPECTRAL IMAGES	poster	36
Lupo	Emanuela	CHARACTERIZATION OF PLASTICS WITH HYPERSPECTRAL METHODS	poster	37
Marini	Federico	SOME COMMENTS ON THE CLASSIFIATION OF HYERSPECTRAL IMAGES	oral	38
Shaver	Jeremy	MULTI-TECHNIQUE IMAGE FUSION AND MULTIVARIATE CURVE RESOLUTION CONSIDERATIONS	oral	39
Burger	James	IMAGE SAMPLING AND DECISION TREES – OPTIMIZATION OF HYPERSPECTRAL IMAGE CALIBRATION MODELS	oral	40

THE IMPORTANCE OF BEING LOCAL: HYPERSPECTRAL NEAR-INFRARED IMAGING APPLICATIONS IN WOOD TECHNOLOGY FOR BIOMASS AND BUILDING MATERIALS

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Wood is used for many purposes: as a building material, for producing all kinds of paper, as a fuel and lately also as biomass e.g in the production refined biofuels. Because of the natural non-homogeneous nature of wood, hyperspectral imaging is more useful than just making integrated spectra of homogenized milled powders. Regions of different chemical and mechanical properties have to be identified to allow an efficient usage of the material. These regions may be visually discernable, but often extra wavelengths in the near infrared are needed.

The lecture discusses two hyperspectral imaging examples: one from biofuels [1] and one from impregnation of wood using linseed oil [2,3]. The complete chemometrical analysis of rather large mosaics is presented. One important and difficult aspect of the analysis is the spectral interpretation.

A helpful tool in imaging is the use of local models. Because of the huge amount of pixels in a hyperspectral image, even small subsets may contain thousands of pixels and allow local chemometrics models. These are sometimes useful for easing the spectral interpretation. It is explained how this is done and also what the limitations are.

References:

[1] Lestander T, Geladi P, Larsson S, Thyrel M, Near infrared image analysis for online identification and separation of wood chips with elevated levels of extractives, Journal of Near Infrared Spectroscopy, in press.
[2] Eriksson D, Geladi P, Ulvcrona T, Near-infrared Spectroscopy for the Quantification of Linseed Oil Uptake in Scots pine (Pinus sylvestris L.). Wood Material Science and Engineering, 6, 1-7, 2011.
[3] Geladi P, Eriksson D, Ulvcrona T, Hyperspectral image analysis for studying wood before and after impregnation, in prep.

AUTHENTICITY OF DDGS - BOTANICAL ORIGIN CLASSIFICATION BY NEAR INFRARED MICROSCOPY

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Recently the complexity of food and feed production systems has increased. In particular feed materials are obtained from new sources or are produced by new technologies. These can have an effect on animal and human health. For these reasons the origin and authentication of feed is very important for food and feed safety. The authenticity and the origin of the products is linked to the quality of feed material. This situation justified the necessity of analytical authentication systems.

Distillers dried grains with solubles (DDGS) are one of the new supplements for animal feed. They are the products of alcoholic distilling obtained by drying solid residues of fermented grains to which pot ale syrup or evaporated spent wash was added. There are two main sources of distillers grains, the traditional source from brewers, where beverage ethanol is produced, and the growing source from fuel-ethanol plants. DDGS are introduced in the animal food chain because they are characterised by their high nutrient content (proteins, fat), since grain constituents other than starch are concentrated in the distillation residues. However, nutrient content depends directly of the cereal source of the DDGS. The most extended DDGS are the ones from corn but also is possible to find DDGS from wheat, barley or mixes. These DDGS present different nutritional composition and for this reason the authentication is important. In this study, DDGS samples from corn, wheat, barley and mixes have been analysed by Near Infrared Microscopy using NIR mapping, obtained 600 spectra per sample. The near infrared microscopy is a simple and fast technique to authenticate the botanical origin of the DDGS. In this study discrimination model between DDGS of corn, wheat and mixes has been developed.

Acknowledgement: The authors wish to acknowledge the help of Nanta S.A. Madrid, and Servizo de seguridade alimentaria nas productions ganadiras (Xunta de Galicia) for providing samples with different botanical origins.

NEAR-INFRARED HYPERSPECTRAL IMAGING AND MULTIVARIATE IMAGE ANALYSIS TO CHARACTERISE *FUSARIUM* SPECIES ON GROWTH MEDIA

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Near-infrared (NIR) hyperspectral imaging for use in microbiological applications is gaining popularity, but is mostly applied to detection of microorganisms on food and agricultural products. Only two applications regarding the identification and differentiation of microorganisms on growth media by NIR hyperspectral imaging have been reported. The identification of *Campylobacter* from non-*Campylobacter* species was evaluated in the wavelength range 400-900 nm with accuracies between 97-99% [1]. Another study investigated the use of hyperspectral imaging for the differentiation of toxigenic fungi in the wavelength range 450-900 nm and reported classification accuracy of 97.7% [2]. Both studies attributed their classification accuracies to two and three visible wavelengths, respectively. No imaging work regarding growth and growth characteristics of fungi or bacteria has been investigated using the NIR region. Conventional growth and kinetic studies involve the use of classic microbiological techniques coupled with measurements from microscopes and time lapse cameras; cytochemical processing and photo microscopy; and enzyme assays. These are painstaking and time consuming. The aim of this work was thus to study the growth and growth characteristics of three *Fusarium* spp. on growth media using NIR hyperspectral imaging and multivariate image analysis (MIA).

NIR hyperspectral images of colonies of three *Fusarium* spp. were collected at regular time intervals after inoculation to follow their growth. Using classification gradients, it was possible to visualise growth characteristics within each colony. Growth zones were identified in the classification images that could be correlated to different phases of mycelium development during growth. These zones were segmented and the averaged spectra evaluated. Three spectral bands, *i.e.* 1166 nm, 1380 nm and 1918 nm were prominent in the multiplicative scatter corrected and Savitzky-Golay second derivative spectra. These indicated chemical changes, associated with carbohydrates (1166 and 1380 nm) and protein (1918 nm), that occurred as the mycelium grew and matured. The protein band was more prominent in the older more mature fungal material while the younger material was characterised by the carbohydrate spectral band. Using score images it was possible to construct growth curves for each species. This was done by the summation of mycelium pixels at each time point. These curves showed the four phases of growth associated with microbial growth, *i.e.* lag, exponential, deceleration and constant growth. Pixels in the individual growth zones were summed and plotted versus time. These depicted how the zones differed in terms of growth, onset of growth and proliferation. This work would not have been possible with bulk NIR spectroscopy and illustrates the advantage of NIR hyperspectral imaging. The use of the NIR region, together with classification images, allowed visualisation of specific growth zones. Growth curves, usually complicated to construct, could be plotted much easier by summation of pixels over time. Mean spectra indicated differences in carbohydrates and protein as mycelia matured.

References:

[1] S. Yoon, K. Lawrence, J. Line, G. Siragusa, P. Feldner, B. Park, W. Windham, Sens. Instrum. Food Qual. Saf., 4 (2010) 35.
[2] H. Yao, Z. Hruska, R. Kincaid, R. Brown, T. Cleveland, Sens. Instrum. Food Qual. Saf., 2 (2008) 215.

ASSESSMENT OF BISCUIT MOISTURE AND BISCUIT BROWNING

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A fast, non-destructive, versatile method for assessing biscuit quality is presented. The method integrates color (or browning) and moisture assessment with dimensional measurements. In the quality control function of biscuit production this information is important to optimize production processes and to assure quality of the final product.

Spectral imaging and analysis of one biscuit is done in a few seconds. The imaging system, VideometerLab (www.videometer.com) captures 18 high resolution spectral images in the range 400-1000 nm. Acquisition is band-sequential and performed by LED strobing into an integrating sphere illumination geometry. The spectral image will contain a NIST calibrated reflectance spectrum in every pixel.

Biscuit color is estimated either in CIELAB coordinates, or as a browning index. Both representations may be estimated in both the biscuit center region and in the edge/corner region. CIELAB coordinates are spectrally reconstructed from the reflectance spectra, and the baking index is constructed using a normalized canonical discriminant analysis.

A biscuit moisture model has been built on regional spectral imaging features through stepwise feature selection and linear regression towards conventional weight moisture measurements. The data set includes biscuits from different lines and both hot and cooled biscuits. Within the relevant humidity range 1%-3% we obtain a RMSEP of 0.14%.

Dimensional measurements relates to the packaging of the biscuits and consist of height and lateral dimensions, e.g. length and width, and height.

Acknowledgment: The author would like to thank Mr. Jean-Paul Thys for acquiring the images.

References:

[1] Videometer A/S, URL: http://www.videometer.com.
[2] Carstensen, J.M., Folm-Hansen, J. (2003), An apparatus and a method of recording an image of an object. Patent family EP1051660, patent application filed 1998.
[3] M. E. Hansen, B. K. Ersbøll, J. M. Carstensen, A. A. Nielsen (2005), Estimation of critical parameters in concrete production using multispectral vision technology, in: Lecture Notes in Computer Science, LNCS3540, Lecture Notes in Computer Science, Informatics and Mathematical Modelling, Technical University of Denmark, DTU, Building 321, DK-2800 Kgs. Lyngby, 2005, pp. 1228–1237.

IN VITRO STUDY OF UPTAKE AND INTERNALIZATION OF OXIDE NANOPARTICLES IN THE CELL NUCLEUS BY RAMAN MICROSPECTROSCOPY AND MULTIVARIATE CLASSIFICATION

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Inhalation of nanoparticles is of major concern since it is associated with adverse health effects. Conventional methods to study interaction of nanoparticle with cells rely on labelling techniques, where either the particles are selectively tagged with tracer molecules, or cells are selectively stained. These methods require extensive sample preparation, and are intrusive in the sense that they intrinsically modify the surface properties of the nanoparticles, or the cellular environment which may lead to biased results. Here, Raman microspectroscopy – a label-free technique which requires no extensive sample preparation - coupled with multivariate classification is employed to measure the spatial distribution of oxide nanoparticles inside living lung epithelial A549 cells. The cells were exposed to titania (TiO_2) nanoparticles and goethite (FeOOH) nanoparticles in vitro. Employing transmission electron microscopy it is found that after long-time incubation (48 h) a small fraction of nanoparticles are internalized inside the cell nucleus. Raman microspectroscopy and multivariate classification with partial least squares discriminant analysis (PLS-DA) are used to unambiguously prove that nanoparticles are located inside the nucleus. In addition, it is shown that Raman microspectroscopy can be used to readily classify mixtures of internalized TiO_2 and FeOOH nanoparticles inside cells based on their intrinsically different phonon bands.

HYPERSPECTRAL IMAGING FOR THE IDENTIFICATION AND AGE ESTIMATION OF BLOOD STAINS AT THE CRIME SCENE

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Blood traces can play a major role in forensic investigations, as they can be used both to identify people and for crime reconstruction purposes. In addition, it has recently been shown that blood stains can give information about the moment a crime was committed. We demonstrated the possibility to estimate the age of a blood stain using hyperspectral imaging.

When blood exits the human body, oxyhemoglobin oxidizes into methemoglobin, which in turn denatures into hemichrome. This causes a color change from red to brown, which we measured with visible hyperspectral imaging. We were able to identify blood non-destructively, using a multi-component fit of the hemoglobin derivatives [1]. In addition, the relative amount of these derivatives gives an indication of the age [2]. For blood on dark backgrounds, which absorb most of the visible light, we successfully used NIR spectroscopy for the same tasks [3].

Within the project "CSI The Hague", the "CSI lab" was created at the Netherlands Forensic Institute; a test laboratory with a mock crime scene, offering great opportunities for testing new detection techniques. Within this scene, red wine, lipstick and several blood stains of different ages were deposited. Using hyperspectral imaging, we successfully captured the entire crime scene and automatically localized fresh and old blood stains within the scene (

Figure **1**).

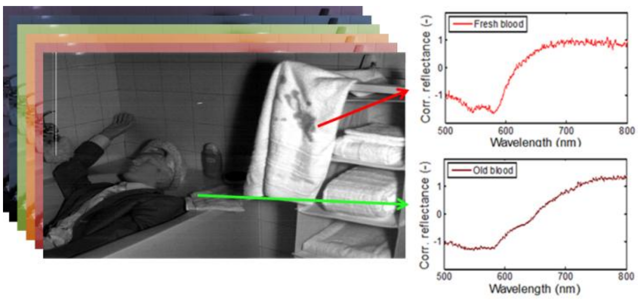

Figure 1 Hypercube showing a mock crime scene and the corrected reflectance spectra of fresh and old blood stains within the scene

Applied in forensic casework, these results could be used to verify suspects' or witness' statements regarding the moment of the crime. Because hyperspectral imaging is non-destructive, all traces are preserved for subsequent analysis in the forensic lab e.g. for DNA analysis.

References:
[1] G. J. Edelman, T. G. van Leeuwen, and M. C. G. Aalders, Hyperspectral imaging of the crime scene for the automatic detection and identification of blood stains, Forensic Science International, Submitted (2012).
[2] G. J. Edelman, T. G. van Leeuwen, and M. C. G. Aalders, Hyperspectral imaging for the age estimation of blood stains at the crime scene, Forensic Science International, (2012).
[3] G. J. Edelman, V. Manti, S. M. van Ruth, T. G. van Leeuwen, and M. C. G. Aalders, Identification and age estimation of blood stains on colored backgrounds by near infrared spectroscopy, Forensic Sci. Int., In press (2012).

NIR HYPERSPECTRAL IMAGING APPLIED TO CLASSIFICATION OF OAT AND GROAT KERNELS

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A procedure to classify oat and groat kernels based on coupling hyperspectral imaging (HSI) in the near infrared (NIR) range (1006-1650 nm) and chemometrics was designed, developed and validated, in order to define a new method that can be implemented for both grain quality control and sorting strategies. In fact, according to market requirements, the amount of groat, that is the hull-less oat kernels, is one of the most important quality characteristics of oats. Hyperspectral images of oat and groat samples have been acquired by using a NIR spectral camera (Specim, Finland) and the resulting data hypercubes were analyzed applying Principal Component Analysis (PCA) for exploratory purposes and Partial Least Squares-Discriminant Analysis (PLS-DA) to build the classification models to discriminate the two kernel typologies. Results showed that it is possible to accurately recognize oat and groat single kernels by HSI in the NIR range (prediction accuracy was almost 100%). The study demonstrated also that good classification results could be obtained using only three wavelengths (1132, 1195 and 1608 nm), selected by means of a bootstrap-VIP procedure. The developed method based on HSI can be utilised for quality control purposes or for the definition of innovative sorting logics of oats. NIR hyperspectral imaging has also big potentiality to be used as an objective and non-destructive method for classification of oat and groat.

NORMALIZED CDA FOR FAT/MUSCLE SEGMENTATION IN SALAMI

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Salami meat and fat color are two of the most important quality parameters for attracting consumers. Several composition, process, and storage parameters influence the meat and fat color changes, e.g. meat type, muscle /fat distribution, herbs, fermentation culture , storage time and temperature.

The aim of this work was to assess the meat color and progress of the ripening of germen type dry fermented salami. A major task in this assessment is the segmentation of muscle and fat. Since both of these classes will be effected by color change, then the segmentation has to be robust to this variation.

In this presentation we compare the use of standard canonical discriminant analysis (CDA) to normalized CDA or nCDA. Both techniques are supervised and painted regions of muscle and fat are provided. The methods are optimized and compared using the maximum Rayleigh quotient,.The nCDA method chooses optimal band normalization on the pixel level and performs a CDA on the normalized pixel values. The nCDA obtains more than 8 times improvement in Rayleigh quotient, and the segmented images also look more correct.

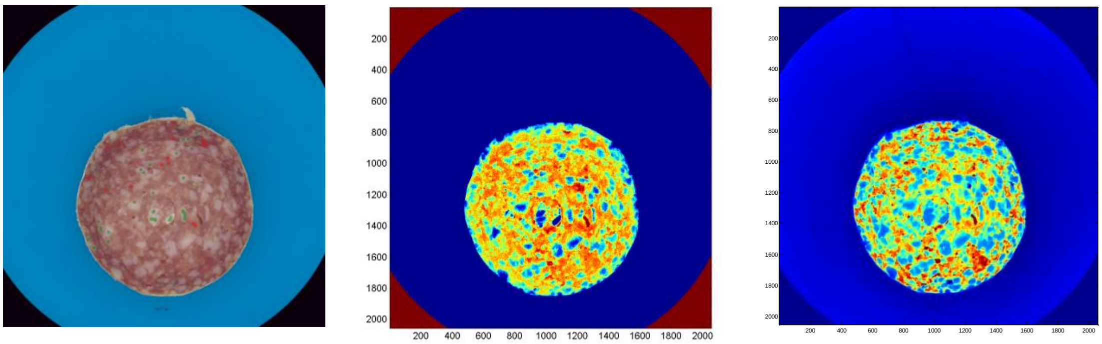

Figure 1 Salami slice (left), CDA based segmentation (middle), and nCDA based segmentation (right)

INTERACTIVE HYPERSPECTRAL APPROACH FOR EXPLORING AND INTERPRETING DESI-MS IMAGES OF CANCEROUS AND NORMAL TISSUE SECTIONS

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Desorption electrospray ionization (DESI) is an ambient mass spectrometry (MS) technique that can be operated in an imaging mode. It is known to provide valuable information on disease state and grade based on lipid profiles in tissue sections. Comprehensive exploration of the spatial and chemical information contained in 2D MS images requires further development of methods for data treatment and interpretation in conjunction with multivariate analysis. In this study, we employ an interactive approach based on principal component analysis (PCA) to interpret the chemical and spatial information obtained from MS imaging of human bladder, kidney, germ cell and prostate cancer and adjacent normal tissues.

Normal and tumor human tissue sections were imaged using a commercial LTQ linear ion trap mass spectrometer and a lab-built prototype DESI-MS ion source. Experiments were carried out in the negative ion mode, using a 5 kV spray voltage, a flow rate of 1.5 μL/min, and 150 psi nebulizing gas (N_2) pressure. The spray solvent was acetonitrile:water (50:50 v/v). Mass spectra were acquired over the range *m/z* 150-1000. For each DESI-MS image, the information was coded using the corresponding data hypercube. Reduction of the spectral variables (1:4) by a consecutive-window averaging algorithm, normalization with respect to the total ion current (TIC) and column-centering were performed. Multivariate analyses were carried through in-house Matlab routines.

This multivariate strategy facilitated characterization between tumor and normal tissue by comparing the lipid information with pathological evaluation of the same samples. Some common lipid ions, such as those of *m/z* 885.5 and *m/z* 788.5, nominally PI (18:0/20:4) and PS (18:0/18:1), as well as ions of free fatty acids and their dimers, appeared to be highly characterizing for different types of human cancers, while other ions, such as those of *m/z* 465.5 (cholesterol sulfate) for prostate cancer tissue and *m/z* 795.5 (seminolipid 16:0/16:0) for germ tissue, appeared to be extremely selective for the type of tissue analyzed. These data confirm that lipid profiles can reflect not only the disease/health state of tissue but also are characteristic of tissue type. The interactive strategy presented here – based on a brushing approach – is particularly useful to visualize the information contained in hyperspectral MS images by automatically connecting regions of PCA score space to pixels of the 2D physical object. The procedures developed in this study consider all the spectral variables and their inter-correlations, and guide subsequent investigations of the mass spectra and single ion images, allowing one to perform thorough characterizations of different regions of any DESI-MS image.

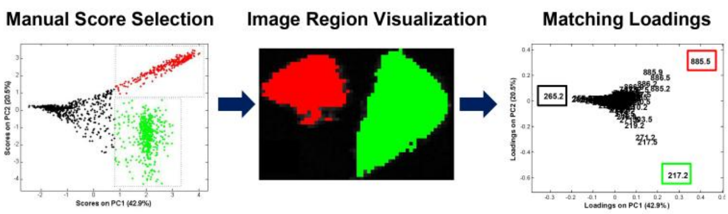

Figure 1 Interactive brushing approach for DESI-MS image characterization

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IDENTIFICATION OF TREE SPECIES IN MULTISPECTRAL IMAGES

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Multispectral imaging exploiting remote sensors has become a widely used tool for the analysis of vegetation in agriculture and forestry. Sub-meter spatial resolution of multispectral images obtained from sensors deployed in aircraft facilitates forest inventory on the individual tree level. One of the most important inventory tasks is species identification. It can be solved by classification of pixels related to the individual tree, containing light reflectance values from spectral bands in visible light and near infrared regions. Individual trees should be delineated beforehand to perform that. This can be done exploiting LiDAR data, if available, or by finding shades between tree crowns in multispectral image. Solution of this task is not discussed here. Instead, methods for identification of tree species are analyzed on the basis of available field data containing coordinates of tree tops and species information.

Analyzed multispectral images were obtained using a hyperspectral imager CASI–1500 from ITRES Research in June, 2008 by flights over the area close to Cesis, Latvia, and provided by the Institute for Environmental Solutions (IES, see www.videsinstituts.lv). 270 individual trees from 5 specific species of interest were located in the same area by the field work. Data acquisition conditions were favorable for classification: analyzed data were obtained during one flight; all classified trees were located in sunlit areas; viewing angle was close to nadir. Spatial resolution of the image was 0.5 m × 0.5 m per pixel, imager was configured to combine data into 13 spectral bands with wavelengths from 400 nm to 970 nm. Envelopes of 20 sunlit pixels from the vicinity of the top of each tree were formed and analyzed.

Several classification methods were considered, including *k*-nearest neighbors, support vector machines (SVM), and Bayes approach [1]. Classification accuracy was tested on the basis of available field data, excluding trees used for training. SVM approach was dismissed as the analysis conditions did not facilitate it. K-nearest neighbors' method provided moderate accuracy. It was found that Bayes approach provided the best results and can be recommended for solving the tree species identification task. It was adapted to the task (equal prior probabilities were assumed as there was no information available about them) and further elaborated to achieve several enhancements [2]. Classification of individual pixels (with later use of a majority vote) and the mean vector of the envelope were considered and both found applicable (the first case providing slightly higher accuracy but the second one giving speed enhancement). The best results were obtained using a pixel-level Bayes classifier with two stages: 1) creating clusters for each species on the basis of the classifier designed from relatively small initial training sets of trees from each species of interest; 2) re-design of the classifier using parameters (mean vector and covariance matrix) of the clusters and performing a second stage on the basis of the obtained more precise classifier. Mean overall accuracy of more than 97% was achieved when the number of trees in the design set of each class was at least 10. However, significantly lower accuracy was observed in particular worst cases, and it was concluded that a careful selection of initial design sets is needed to avoid these. Rules for the selection of design sets were formulated and a parameter characterizing diversity of these sets proposed. By checking the value of this parameter and dismissing design sets with low diversity, more stable classification results were obtained. Another possibility to increase robustness of the classifier was proposed, based on performing multiple classification attempts using different training subsets of trees, and a majority rule to derive the final decision. This approach provided an additional increase of the mean overall accuracy as well.

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IDENTIFICATION OF FOREST AREAS AND FOREST INVENTORY PARAMETERS IN MULTISPECTRAL SATELLITE IMAGES USING SUPERVISED CLASSIFICATION METHODS

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Forest is one of the most important natural resources in Latvia, so precise information about condition of the forests is crucial for sustainable management and planning of the environment. Artificial earth satellites provide an opportunity to obtain multispectral data about vast areas, the examination of which in presence requires financial and time resources. Many automatic classification methods have been developed to classify multispectral satellite data for land cover identification. The aim of this research is to estimate forest areas and forest inventory parameters (dominant tree species and stand volume) in the research area in Latvia using supervised classification methods. Classification was performed using two satellite image sets: Landsat ETM+ and RapidEye images of year 2011. RapidEye images provide higher spatial and radiometric resolution while Landsat ETM+ covers wider part of electromagnetic spectrum. Sample data for statistical classifier training were selected automatically using National Forest inventory plots in shapefile format.

Some of the most popular supervised classifiers were tested for land cover and tree species identification: k – nearest neighbours (kNN), which is widely used for forestry applications [1], [2], Gaussian maximum likelihood classifier and support vector machine (SVM). Several multispectral satellite band image transformations were tested as input data for classifiers. Results show that overall accuracy of all classifiers is similar, while multispectral image ratios improve accuracy. Accuracy of the classification was evaluated at pixel level using confusion matrix and related characteristics. Overall accuracy for land cover classification was 94%, but for tree species approximately 69%. Results could be improved using point-like sample plots with precise geographic coordinates.

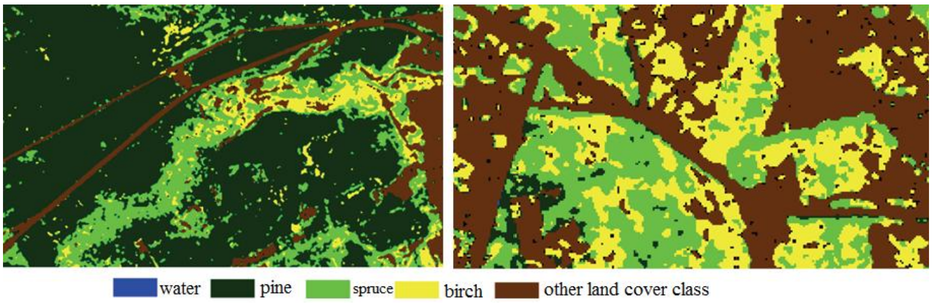

Figure 1 Fragments of the resulting tree species and land cover map (obtained using k – nearest neighbours method)

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QUANTIFICATION SALAMI COLOUR AND TEXTURE CHANGES

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Salami meat colour and fat are two of the most important quality parameters for attracting consumers [1]. Several storage and composition parameters influence the meat and fat colour changes, e.g. age, size, temperature, meat type, bacteria culture and herbs.

The aim of this work was to assess colour, texture and the progress of ripening of German type dry fermented salami. During ripening, three visual changes take place:

1. Texture change where muscle and fat becomes more emulsified (combined)
2. Colour change
    a. general darkening of the meat
    b. gradient from edge to center

It is demonstrated how spectral images can be used to follow and discriminate between different salami formulations throughout the ripening period.

Spectral images were generated using a VideometerLab instrument, which is a focal plane type instrument [2] using LEDs placed in an integrating sphere and a 5 megapixel camera to generate spectral images (375-970 nm).

Figure 1 Salami slice on date of production (left), Salami on day 28 (middle) and a color map showing progress of ripening on day 28 (right)

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MONITORING OF MOISTURE CONTENT AND BASIC SPECIFIC GRAVITY IN BLACK SPRUCE LOGS USING A HANDHELD MEMS-BASED NEAR-INFRARED SPECTROMETER

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Our study presents a test of a handheld micro-electro-mechanical system (MEMS) based near-infrared (NIR) spectrometer to measure moisture content and basic specific gravity over black spruce frozen and unfrozen logs. MEMS-based spectrometers offer significant advantages such has high portability and high signal-to-noise ratio [1, 2], which are key drivers in developing new applications that were previously either technically-impossible or not economical [3]. The spectra were acquired on sapwood and heartwood as well as tangential and transversal log sections. Partial least square regression is used to calibrate and validate the models that relate NIR spectral data to the log property. Temperature-specific and generalized models were developed and they gave similar prediction accuracy. The generalized models have however the advantage of handling measurements from both frozen and unfrozen logs, as presented in Figure 1. From Figure 1, it does not seem that log freezing conditions influence the prediction of moisture content and basic specific gravity using NIR spectra.

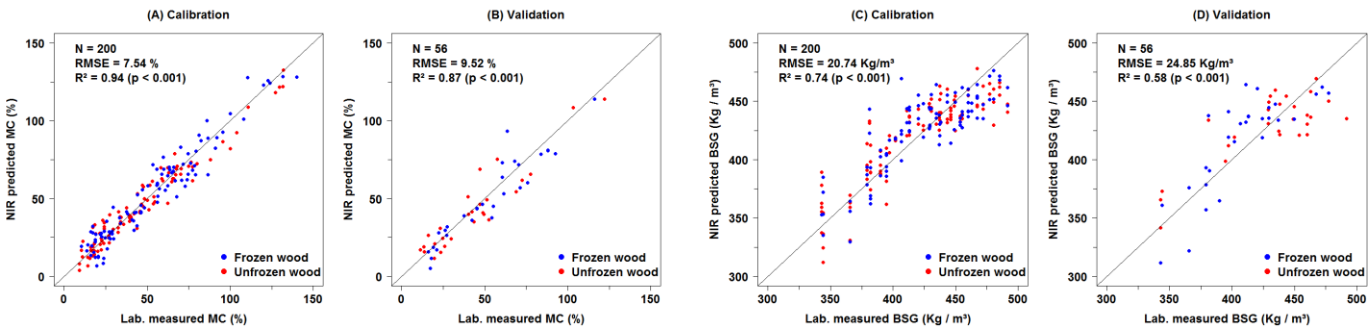

Figure 1 Generalized PLS models for the prediction of moisture content (MC) [A,B] and basic specific gravity (BSG) [C,D] using NIR spectra obtained from unfrozen and frozen black spruce logs. Models were built using 16 components and with the mean spectra collected on sapwood and heartwood over the transversal section

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USE OF HYPERSPECTROGRAMS FOR DATA COMPRESSION AND INFORMATION EXTRACTION FROM HYPERSPECTRAL IMAGES

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When using HyperSpectral Imaging (HSI) techniques, a wide amount of data can be easily acquired in very short times, and generally without the need of sample preparation. The key step is the extraction of the useful information contained in each hypercube, which is a three-dimensional array generally consisting in more than one hundred of congruent images, each one often composed by tens of thousands of pixels, recorded at different wavelengths and stacked to each other. Therefore, in order to properly exploit the great potentialities offered by this analytical technique, efficient chemometric strategies must be developed to deal proficiently with datasets that can easily reach enormous dimensions. The compression of useful information into an optimized set of few parameter values, in fact, is essential for analysing datasets formed by a large number of images, as well as for enabling on-line monitoring.

In this context, we propose a strategy to reduce significantly both the dataset size and the required computational load, while preserving at the same time the useful information contained in the dataset. This procedure is derived from the colourgrams approach, already developed by some of us for the elaboration of RGB images [1, 2]. It essentially consists in compressing the useful information contained in each hypercube into a one-dimensional signal, named hyperspectrogram, which is composed by the frequency distribution curves of score and residual vectors obtained by applying PCA to the unfolded hypercube data. In this manner, the hyperspectrogram-based approach allows to compress the millions of data of the original image into a vector composed by few hundreds of data. Hyperspectrograms can then be used as a compact set of descriptors and further analysed by common multivariate analysis methods for data exploration, classification or calibration. Moreover, using proper variable selection methods, hyperspectrograms can be further compressed to few significant descriptors, allowing to extract only the specific features that are useful to solve the problem at hand. Additionally, these features can be projected back into the image space, allowing to perform a visual evaluation of the choices made by the feature selection method.

Examples of applications of the hyperspectrogram-based approach to hyperspectral images of food samples in the Vis and NIR ranges demonstrate the usefulness of this approach.

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SKIN HEMOGLOBIN ASSESSMENT BY SPECTRAL IMAGING IN VISIBLE RANGE

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Optical imaging technologies are used for non-invasive assessment of skin blood supply. Laser Doppler perfusion imaging and laser speckle imaging are commercially available techniques for mapping of microvascular perfusion in tissue [1]. Multi-spectral imaging (MSI) has shown potential for mapping of skin chromophores, e.g. oxy-/deoxy-hemoglobin and melanin [2]. Such mapping ensures reliable non-invasive evaluation of skin condition and can be used for evaluation of vascular malformation treatment [3].

Multi-spectral imaging was provided by halogen lamp ring-light illumination and liquid crystal tunable filter (LCFT) acquiring 51 images in spectral range 450 – 950 nm with spectral resolution 10 nm. Visible spectral range 500 – 700 nm was selected for evaluation of skin chromophore changes. The system was approbated in laboratory by arterial and venous occlusion tests. Clinical trial was performed by monitoring vascular malformations laser treatment. For example, color images of telangiectasia before and after treatment and corresponding chromophore maps are shown in Figure 1.

Besides, RGB imaging system for mapping and monitoring of hemoglobin distribution in skin has been designed and tested. RGB sensor can be regarded as a simple and fast MSI device acquiring three spectral (red (R), green (G) and blue (B)) images simultaneously. In combination with specific narrow-band spectral light sources RGB imaging could become competitive for some specific applications, including the assessment of skin chromophore concentration [4 5].

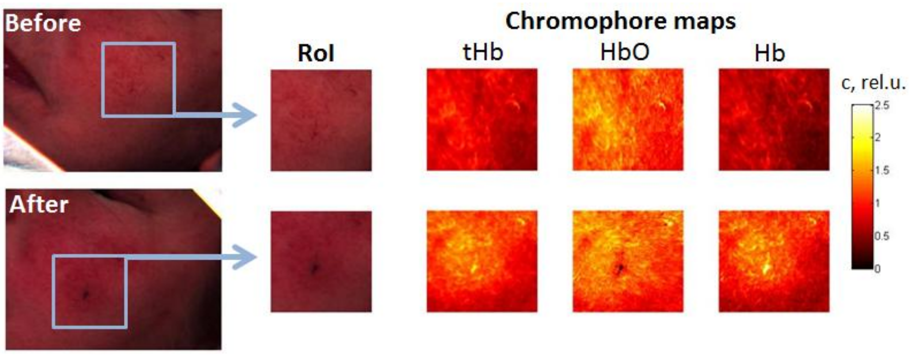

Figure 1 Telangiectasia before and after laser treatment: color images and chromophore maps (tHb – total hemoglobin, HbO_2 – oxy-hemoglobin and Hb – deoxy-hemoglobin) of region of interest (RoI)

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MULTIVARIATE CURVE RESOLUTION AND ROTATION EVALUATION ON REMOTE SENSING HYPERSPECTRAL IMAGES

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MCR-ALS is applied to three different remote sensing hyperspectral images which were obtained by the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) operated by NASA and they are in public databases [1]. The first one is a reference image of Cuprite, Nevada, in 1997, which was with 224 spectral bands over 400-2500nm. The size of the data set is 614×512 pixels. The Cuprite area is arid with a small amount of vegetation cover, and has rock exposures comprising alteration zones characterized by the occurrence of key indicator minerals. The second image is from a remote sensing test site on the bay of San Francisco, a few kilometers north of the city of Mountain View, California. The site includes the Naval Air Station Moffet Field, agriculture fields, water ponds, salt banks, and man-made constructions such as several airplane hangars which today are museums. It is ideal for water variability, vegetation and urban studies. The third image is taken at the airport of the airfield in San Diego, California. It has size of 400×400, and it has 224 spectral bands over 400-2500nm. The study of this area includes vegetation, tarmac and concrete. Minerals in the first image, water, vegetation and urban in the second image and airplanes in the third image are investigated in the hyperspectral images. MCR-ALS is tested to analyze and resolve these areas with different characteristics. Results achieved show that MCR-ALS performs well for the resolution of these hyperspectral images from remote sensing. To check the extent of rotation ambiguities associated to a particular MCR solution under a set of constrains, MCR-BANDS [2,3] was also applied to these datasets and to a dataset which was simulated using three spectral signatures extracted from the 1997 USGS Digital Spectral Library. The maximum and minimum of the relative signal contribution of each resolved pure component together with their corresponding spectra were estimated and their distribution maps (images) compared. The obtained results confirm that MCR-BANDS results did include those profiles resolved by MCR-ALS and also by some other spectroscopic image analysis methods like VCA [4] and MVSA [5]).

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EVALUATION OF CHEMICAL CHANGES IN NIR HYPERSPECTRAL IMAGES OF CEREALS USING CLASSIFICATION GRADIENTS

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Near infrared hyperspectral imaging (NIR-HSI) is a powerful technique for studying chemical changes in biological materials, i.e. heterogeneous samples. The non-destructive nature of NIR-HSI allows for the same sample to be analysed and evaluated over time. This enabled the study of movement of conditioning water in wheat kernels [1] and the viability of wheat, barley and sorghum kernels [2]. Images were collected using a sisuCHEMA SWIR hyperspectral camera. This pushbroom imaging system collects spectra from 1000-2498 nm with 6-7 nm resolution. The hypercube dimensions varied depended on the lens used, spatial dimensions and field-of-view. Internal dark and white reference standards were used for image calibration and the Evince software package for data analysis.

Interpretation of principal component analysis (PCA) score images and plots were difficult due to no clear clustering in the score plots. This is often seen for biological samples in spite of known biological changes to have taken place in the samples analysed over time. It was realised that it was easier to follow biological changes over time using ‘classification gradients’. Classification gradients were defined by dividing the scores range for a specific PC into between four and six successive groups starting with the negative score values. This was done for each PC in both the studies. The first selected group thus consisted of pixels with the most negative score values for the specific PC and the last group consisted of pixels with the most positive score values. Each of these groups was assigned a distinct colour in the score plot which was subsequently projected onto the score image to create a classification image. These classification images allowed the score image to be interpreted more efficiently in terms of chemical changes over time.

Classification gradients allowed identification of the underlying source of variation explained in each PC, i.e. movement of moisture in wheat grains differing in hardness and detection of germination (non-viability) in cereal grains. Using classification gradients allows, in addition identification of physical effects that could affect the results and subsequent separation of these effects (scattering) and chemical differences. Having both spatial and spectral aspects of the images contributed to these conclusions. Visualisation of spatial dimensions, where each pixel represent a complete spectrum, gives NIR-HSI (in combination with chemometrics) a huge advantage over mere bulk NIR analysis in terms of interpretation of data. The use of classification gradients simplified the interpretation.

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HYPERSPECTRAL SCATTER IMAGING FOR APPLE QUALITY EVALUATION DURING SHELF-LIFE STORAGE

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After harvesting, apples are stored under controlled atmosphere for several months before being supplied to the consumer. Storage conditions have a strong influence on biochemical reactions that occur in apples and affect the fruit quality. There is always a need in fast and non-destructive techniques for determination of internal fruit quality for online sorting and grading the fruits after being stored.

Optical measurement techniques, such as Visible and Near Infrared spectroscopy have been applied as non-destructive methods for monitoring the quality attributes of fruits. However, these methods are often not robust due to complex nature of fruit tissue and interaction of incident light with fruit sample involving both absorption and scattering of the light [1]. The light scattering is primarily considered due to physical characteristics of apple fruit (e.g., firmness, cellular structure, density, porosity), whereas light absorption is related to the chemical constituents (e.g., soluble solid content, organic acids). As both the chemical and physical properties of the apple fruit are of interest, it would be interesting to extract thesefrom the spectroscopic spectra.

This can be obtained by combining multiple spatially resolved spectral measurements with light propagation models. In spatially resolved spectroscopy, light of constant intensity illuminates the sample and multiple detectors at different distances are used to record the scattering profile of the light [2]. This is typically done with fiber-probes that are placed in contact with the sample. Although this contact guarantees collection of the diffusely reflected light at the desired positions, it makes this technique less applicable for online sorting and inspection of fruits at desired industrial high speed. Therefore, the hyperspectral scatter imaging technique has been elaborated to perform contactless spatially resolved spectroscopy.

In this study, the potential of hyperspectral scatter imaging for contactless monitoring of the optical properties of apple fruit stored at optimal and brown inducing storage conditions has been studied for better understanding the changes in microstructure and composition properties of apples during shelf-life storage. Results show that the hyperspectral scatter imaging technique has a potential to be used as contactless and rapid method for online quality determination of apple fruit at different storage stages.

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FOUR SPECTRAL BAND VIDEO-IMAGING DEVICE FOR SKIN DIAGNOSTICS

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In this study simple and inexpensive multispectral device was developed. The commercially available digital video microscope (*Dino-Lite*) was modified for skin pathology diagnostics. The white light emitting diodes (LEDs) were replaced with 4 blue (450 nm), 4 green (545 nm), 4 red (660 nm) and 4 infrared (940 nm) LEDs.

The developed software and system modification allows obtaining 4 different spectral images within few seconds, and calculating maps of 3 skin pathology diagnostic parameters (erythema and bilirubin indexes, and melanoma diagnostics parameter- C43 indicator) by simple manipulations with source images in real time (Figure1).

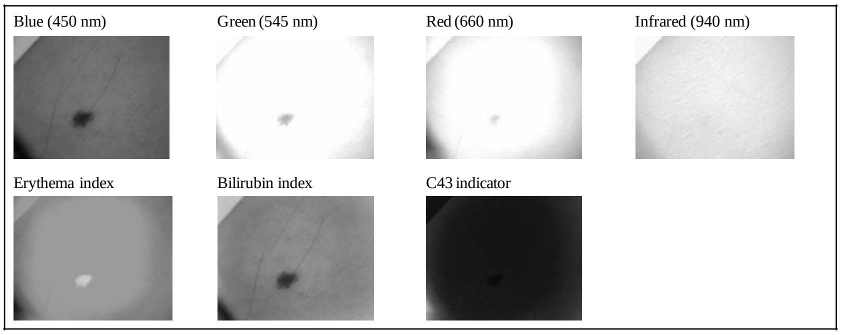

Figure 1 Spectral images and real time mappings of a pigmented nevus using the developed software

Since the blood absorption spectrum is known [1], erythema index was calculated using following expression:

$$E = I_{660}/I_{545}. \quad (1)$$

For bilirubin index [2] the following formula was used:

$$B = I_{450}/I_{660}, \quad (2)$$

To calculate melanoma diagnostics parameter *p*, mathematical expression for the optical density [3] was converted for intensities of diffuse reflected light from the skin:

$$p = I_{545} / (I_{660} \cdot I_{940}), \quad (3)$$

The second off-line software was developed for detailed skin chromophore analysis. In addition, concentration maps of melanin, oxyhemoglobin and deoxyhemoglobin can be obtained using regression analysis. The developed application was tested clinically on more than 20 volunteers with different vascular and pigmented skin malformations.

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XRF HYPERSPECTRAL MAPPING OF PAINTED SURFACES FOR PAINTING CHARACTERISATION – A MULTIVARIATE EXPLORATORY APPROACH

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In the last decades, *in situ* non-invasive analytical techniques have been widely deployed for preliminary screening of areas of interest on painted surfaces and for identifying suitable sub-areas to be sampled and submitted to deeper laboratory investigations. Among the analytical techniques commonly used for *in situ* investigations of painted surfaces, X-ray fluorescence (XRF) spectroscopy represents one of the most widely applied [1]. This technique permits the identification of different elements present in inorganic compounds, addressing the need to investigate highly complex materials, characterising their local properties and modifications. Furthermore, it is possible to record spectra spanning a surface, obtaining a hyperspesctral XRF map useful for characterise elemental composition of different parts of a sample. Spectra recorded may be affected by unwanted variability, especially horizontal shift of peaks, due to small temperature variations. For this reason, suitable signal processing strategies are profitable.

This research work presents a combined strategy for peak alignment – based on the correlation optimized warping (COW) algorithm [2] – and multivariate treatment of XRF hyperspectral data. In fact, multivariate methods should be considered as the most appropriate approach to extract useful information from elemental analyses, thanks to their capability to account for inter-correlation among variables, which are of high importance for elemental analyses. Despite of this, their application in this field is still not so common.

A methodological approach is presented, which allows spectral profiles to be analysed directly, without computation of derived parameters, by means of principal component analysis (PCA). Inter-correlation among variables is assessed by examination of loadings on the PCs of interest. Furthermore, a graphical representation of the correlation of the spectral variables with a selected one is performed. Such correlation diagrams show the correlation coefficient coded by a colour scale as shadowed area under the average spectral profile and are functional to highlight inter-relations among elements within the spectra considered. This helps to identify and localise multi-element components.

The application of the approach on the famous Renaissance wooden painting "The Ideal City" (Palazzo Ducale, Urbino, Italy) is presented and discussed as a case study.

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A PCA-BASED HYPERSPECTRAL APPROACH TO DETECT EDIBLE MUSHROOMS INFECTED BY MYCOPHILIC FUNGI

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Mycophilic fungi of anamorphic genus *Sepedonium* (telomorphs in *Hypomyces*, *Hypocreales*, Ascomycota) infect and parasitize the fruit bodies (or sporomata) of boleticolous species, forming conidia in the final stage of the infection process [1-3]. The preferred hosts are genera within *Boletales*, such as *Boletus*, which include the most and expensive edible wild-grown mushrooms, *Boletus edulis* and relative group. Infections lead to total necrosis and the formation of large quantities of yellow aleurioconidia [4].

Up to date, *Sepedonium* infections have been evaluated only through macroscopic and microscopic analysis by experts mycologists, but this method can be too expensive, in terms of time, as a routine methodology for industrial purposes. Up to now, no analytical technique has been proposed for the detection of *Sepedonium*, while different applications of hyperspectral imaging (HSI) and chemometrics for monitoring different aspects of mushroom quality have been reported [5-6].

In this study, the potential application of HSI and principal component analysis (PCA) for detection of *Sepedonium* infection on *Boletus edulis* and relative group was investigated.

Hyperspectral images were obtained using a pushbroom line-scanning HSI instrument, operating in the wavelength range between 400–1000 nm with 5 nm resolution. PCA was applied on a training dataset composed by 14 average spectra of normal samples and 14 average spectra of contaminated samples, which were obtained by selecting regions of mushrooms corresponding to the two typologies, respectively, at different points on the mushroom surfaces. It was observed that normal and contaminated tissues were separable on the basis of the score on second principal component (PC 2), while the image background was separated from the mushroom image along the first principal component (PC 1). A supervised rule was then developed to assign spectra recorded on new test samples to each of the two classes, based on the PC scores. This allowed to visualize directly – within false-color images of test samples – which points of the samples were contaminated.

The results achieved might lead to the development of a non-destructive monitoring system for a rapid on-line screening of contaminated mushrooms.

Acknowledgement: DV-Optic Tecnologie d'Avanguardia (Padova, Italy) is gratefully acknowledged for having provided instrumentation use.

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FEASIBILITY OF HYPERSPECTRAL IMAGING FOR PHARMACEUTICAL CLEANING VERIFICATION

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Cleaning verification is routinely conducted in the pharmaceutical industry to verify the cleaning procedure used to remove residues from equipment surfaces. Currently, the reference method employed for cleaning verification involves swabbing the product-contact surfaces and analysis of the swabs by HPLC. Cleaning verification poses a real challenge to the pharmaceutical sector in terms of downtown time and the need for highly trained personnel. Therefore there is a need for a rapid, sensitive on-line detection technique that may detect low concentrations of active pharmaceutical ingredient (API) residues on the equipment [1]. The objective of this study was to evalute the potential of NIR Hyperspectral Imaging (HSI) for cleaning verification in pharmaceutical manufacture equipment. Serial dilutions of caffeine, lactose and caffeine/lactose blends (10:90, 50:50 and 90:10) were used to soil stainless steel coupons. Dried stains were analysed by HSI with the datacubes processed using R software (R Foundation). NIR hyperspectral images were autoscaled and masked to differentiate residues from the stainless steel background (Figure 1). The threshold in the mask algorithm was obtained from the autoscaled distribution of stainless steel pixels (3×Standard Deviation) and was applied at two wavelengths. A pixel count was then obtained per stain concentration level (100-1 ug/mm^2) and the data fitted with a linear model. The squared correlation coefficient (R^2) value of the calibration models was higher than 0.9 in all cases which suggests that concentration of residues on surfaces (ug/mm^2) can be successfully modelled from NIR chemical images. In summary, a simple procedure was developed based on NIR-HSI and image analysis for the quantification of low levels of APIs such caffeine on the surface of stainless steel coupons.

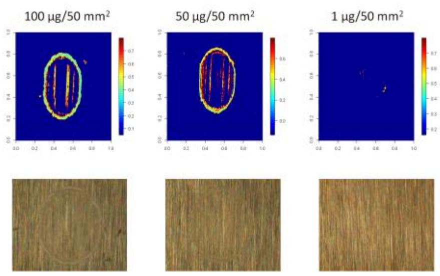

Figure 1 NIR masked images (top) and stereoscope images (bottom) of caffeine (100, 50 and 1 µg/50 mm^2)

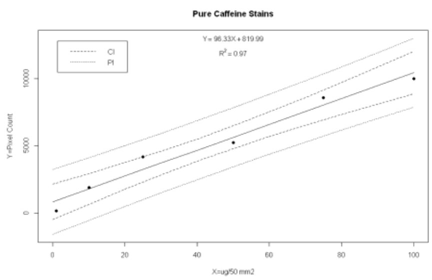

Figure 2 Fitted linear model of pixel count from masked NIR-CI of caffeine versus stain concentration level (ug/50mm^2)

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SPECTRAL CHARACTERISTICS OF IRON ORE MINERALS USING MODIFIED GAUSSIAN MODEL

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Hyperspectral imagery provides the end-user with useful information about mineralogical compositions through a study of their constituent characteristic absorption features. Derivative Analysis followed by smoothing [1] is helpful for identification of absorption bands in the spectrum. Spectral diagnostic interpretation depends on the quantifiable parameters such as band depth, band center and band strength. These parameters represent individual absorption bands as discrete mathematical distributions and facilitate modeling the spectral signatures. Modified Gaussian Model (MGM) [2] is helpful for analysis of Spectral diagnostics and is dependent upon the RMS residual error fit. MGM analysis suggests that the band width depends upon the electronic transition presents in the mineral. Iron spectral signatures are dominated by an absorption features at near 650 to 750nm and 850-1100nm that consists of three overlapping absorption bands caused by the spin allowed electronic transition of Fe^{+2} and Fe^{+3} crystal filed sites [3,4]. XRD/XRF analysis and the spectral diagnostics obtained from hand-held Field Spectro radiometry show compatible results. The research work indicates that Derivative and MGM method are useful and viable method for hyper spectral remote sensing for rocks/ mineral identification characteristics of the minerals.

Acknowledgement: The authors are thankful to Regional Remote Sensing Centre (East), India for their cooperation in field and laboratory data collection and providing the equipment support.

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DEVELOPMENT OF MULTISPECTRAL BIO-MEDICAL IMAGING SYSTEM

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A novel multispectral imaging system for skin pathology diagnostics has been developed. System consists of 4 main parts – processing unit, memory, CMOS image sensor and two LED rings (Figure 1). Multispectral imaging is achieved by spectrally selective illumination using light emitting diodes (LEDs) with central wavelengths 420nm, 540nm, 580nm, 660nm and 950nm, combined with the known spectral R, G and B detection bands of the image sensor. Optical system provides uniform polarized illumination, and image detection via orthogonally oriented polarizer helps to register predominantly the diffuse reflectance of skin. Besides, skin auto fluorescence photo-bleaching rate images and microcirculation perfusion maps are recorded with the same system.

On-board and off-board (external computer) calculations are performed to extract skin parametric maps (oxy- and deoxy-haemoglobin, melanin, bilirubin, etc.) from the obtained spectral images and video-data.

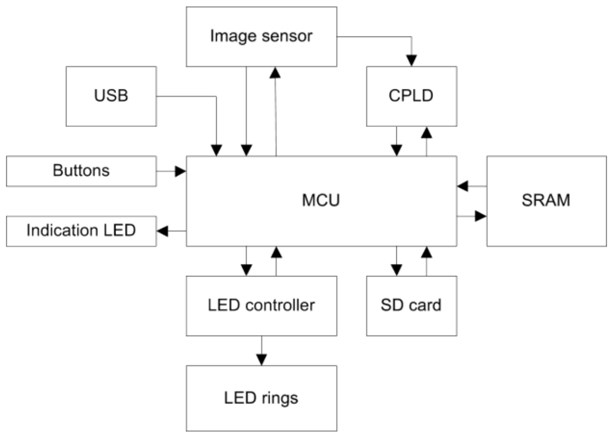

Figure 1 Block diagram of the System

Measurement is done by placing system on skins area of interest and pressing start button. During measurement system goes through three procedures:

1. System captures five RGB images at different LED light sources;
2. System captures B channel video (2 frames per second) for 20 seconds at UV LED illumination;
3. System captures G channel video (15 – 30 frames per second) for 20 seconds at (540 nm) LED illumination.

Acknowledgement: ERDF project "New optical technologies for complex non-contact skin diagnostics" No. 2010/0271/2DP/2.1.1.1.0/10/APIA/VIAA/030.

OPTIMIZED EXTRACTION OF THE ARTERIAL INPUT FUNCTION IN PROSTATE DCE-MR IMAGES BY MULTIVARIATE IMAGE ANALYSIS

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In order to obtain an optimized individual arterial input function (AIF) of the prostate, multivariate image analysis techniques have been applied. A set of 10 patients with potential prostate carcinoma were studied with 3T DCE-MR imaging (3D sEG, TR/TE=6.1/1.7 ms, FA=40º, 3 s/dynamic (non-equally spaced temporal samples), acquisition_time=5'30'', voxel_size=1x1x4 mm, Gd-DOTA=0.2 ml/kg @4 ml/s).

Multivariate Curve Resolution (MCR) has been used to improve previous analyses based on Princiapl Component Analysis. After applying SIMPLISMA, assuming a certain number of perfussion dynamis in the prostate area, MCR was applied imposing non-negativuty restrictions both in the dynamics (spectra) and on the contrast concentrations. The results were enhanced by using Fixed Size Image Window-Evolving Factor Analysis (FSIW-EFA), in order to determine the number of dynamics present in a window. This way, it was possible to determine whether a patient was affected by a prostate tumour, since in this case all four components extracted by MCR have a clinical meaning.

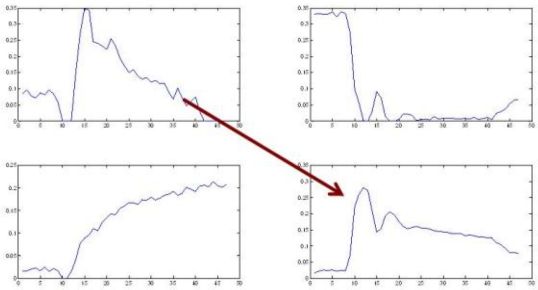

Figure 1 Extraction of the dymamics present in the image: perfusion (affected prostate) (top left), initial stationary state (top right), perfusion (sane prostate) (botton left) and perfusion in the arteries (bottom right)

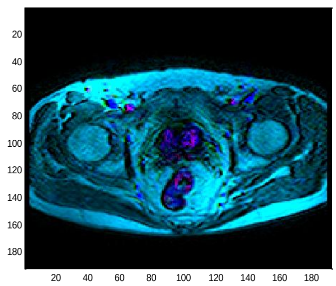

Figure 2 False color composite of the dynamics of interest (affected prostate in purple)

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USE OF NEAR-INFRARED HYPERSPECTRAL IMAGES FOR LOG MOISTURE CONTENT DISTRIBUTION MAPPING

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Various processes in the forest products industry demand accurate estimation of moisture content (MC) of logs. Up to now, hyperspectral imaging systems have been tested to identify compression wood in Norway spruce and Scot pine lumbers [1]-[2] and for estimating density, microfibril angle and stiffness of wood strips of *Pinus taeda* [4]. They were also used to map chemical composition [5] and MC [6] of unfrozen lobolly pine logs. In our study, both frozen and unfrozen logs have been imaged with a *Specim NIR line scan* imaging spectrometer. Frozen logs mimic the winter conditions in a mill yard in Canada. The near-infrared hyperspectral imagery (NIR-HSI) were acquired over logs from one softwood tree species (black spruce (*Picea mariana* Mill.). MC of each image pixel was estimated from the near-infrared spectra extracted from the images using a Partial Least Square (PLS) regression model. The output of this study will provide a non-destructive method to produce a 2D spatial distribution of MC of frozen and unfrozen logs.

Acknowledgement: The authors thank Kathie Phung and Gordon Chow for their technical help. The study was funded by a NSERC Strategic Grant awarded to Leblon et al.

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NON-SCANNING HYPERSPECTRAL FRAME CAMERA FOR INDOOR AND OUTDOOR SPECTRAL IMAGING

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Hyperspectral imaging techniques are used in many scientific and industrial applications. The higher the number of the applications the higher is the demand for rapid, high-quality and easy-to-use data acquisition tools. Nowadays hyperspectral imaging is particularly dominated by scanners for both indoor and outdoor applications. Spectral scanners have successfully mastered many applications, however scanning hyperspectral cameras in certain cases can face limitations in usability, robustness and speed.

Scanning is limited when the test object is randomly changing or rapidly moving in time and space or the user intends to go for a spectral image capturing „walk” without a stabilized camera holder. To go over this limitation complementary spectral imaging techniques are needed to minimize the gap between user demands and technological limitations.

On the basis of research results of the Institute of Laser Technologies in Medicine and Metrology at the University of Ulm, the Cubert-GmbH has developed a hyperspectral frame camera that enables non-scanning hyperspectral imaging. This technical approach targets the mobile and time critical applications both in laboratory and in the field.

This spectral camera behaves like a digital camera with one exception, it delivers a spectrum for every pixel in the Image.

At the present stage of the development the platform provides 140 channels in a spectral range of 400-1000 nm.

This time the spatial resolution is subject to change depending on applications. The camera provides images up to 1.3 MPixel and delivers up to 62,000 unique spectra per second. The camera is able to proceed up to 25 images per second that means it can be used as spectral camcorder. The integration time of one hyperspectral data cube takes 1 ms in an optimal illumination scenario. The dynamic resolution is 14 bit. The whole equipment can be less then 1000 g enabling high mobility and flexibility.

The present development of the camera is focusing on performance optimisation and ergonomic improvements resulting from application priorities. Looking at a long-term scale the development aims to extend the spectral ranges of the camera over 1000 nm.

The platform is open for external research goals, scientific and industrial cooperations and customized solutions can be considered and are welcome. First applications have been implemented for food quality assessment and UAV based airborne imaging.

HYPERSPECTRAL IMAGE ANALYSIS BY ULTRAFAST RAMAN IMAGING

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Ultrafast Raman imaging is a powerful tool for providing spatial and spectral information about the samples analyzed. Thus a confocal Raman imaging system presents a big potential to reduce overall measurement time, since the complete spectral information from all pixels can be acquired in minutes. Time-resolved Raman measurement is especially useful for a fast collection of series of images about the same sample or on several related samples.

The analysis of several Raman images is useful in many instances, such as to study layers from the same sample scanned at different depths, or to identify and quantify constituents in common of several pills from a production line. From a data analysis point of view, simultaneous analysis of several images call for the use of image spectra resolution.

The aim of hyperspectral image resolution methods is to provide distribution maps and pure spectra related to image constituents of a sample from the information contained in the measured raw image. Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) is an iterative resolution method oriented to recover the underlying spectroscopic bilinear model, i.e., concentration profiles (folded back into distribution maps) and pure spectra, by applying constraints related to chemical or mathematical properties of the profiles to be resolved. Single image analysis by MCR is often used, but it may be easily extended to the analysis of multiset structures formed by several images [1,2].

A set of standards and pills images, acquired by Ultrafast Raman imaging at different spatial resolutions, will be submitted to multiset image resolution to obtain quantitative information both at a global and local pixel level. Effect of coupling images with different pixel size in the same analysis will be explored. On the other hand, layers from a scotch sample scanned at different depths are analyzed to achieve a proper description of the heterogeneity of the polymer and the adhesive compound through the different layers [1,3]. Both examples will show the potential of hyperspectral image resolution analysis on ultrafast Raman imaging measurements.

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IMAGE MULTISET ANALYSIS: ENHANCING IMAGE INFORMATION

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Image multiset analysis consists of treating simultaneously series of images having common or related information. The relationship can come from the chemical sample (images collected at different sample depths or positions) or from the chemical problem (images acquired during a process or images used to form a calibration set in a quantitative analysis context). In any of these instances, the simultaneous analysis of these connected images provides more accurate and reliable information than the individual analysis of each of them [1].

Multivariate resolution methods offer a simple framework to accommodate multiset image analysis since only the spectral information among images should be common. As a consequence, images from different morphologies, pixel size, spatial resolution, ... can be analyzed together [2,3].

Apart from the usual examples of multilayer images of the same samples or sets of images obtained to get local and global quantitative information, special focus will be on examples of image multisets oriented to obtain the description of a process and to enhance the spatial resolution of an image measurement by combining shifted images obtained at a low spatial resolution level. The multiset examples presented are formed by IR, NIR and Raman hyperspectral images.

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DEVELOPMENT OF A SYSTEM FOR RAPID SCREENING OF WATER SAMPLES USING NIR CHEMICAL IMAGING

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The overall objective of this research is to investigate the potential use of NIR Chemical imaging (NIR-CI) for rapid screening of water. In this study, a transflectance imaging system was developed for simultaneous imaging of multiple thin layer water samples. In order to demonstrate the potential of this technique, three sample types were investigated: water, glucose and NaCl solutions (both at 1 mol.L-1). Chemical images were obtained using a pushbroom line-scanning instrument, operating in the wavelength range of 870–1720nm with spectroscopic resolution of 7 nm. The effective resolution of the InGaAs detector was 240 x 320 pixels. Principal component (PC) analysis was applied to the chemical images, unfolded along the second spatial axis, and PC score images showed a clear separation of the three sample types along the direction of the fourth PC (Fig.1). Examination of the corresponding PC loading revealed that this separation was largely due to changes in the location of the first overtone of the O-H stretch in the vibrational spectrum of water, arising due to the addition of NaCl or glucose. Further research is required in order to examine the stability of this system, influence of ambient conditions and limits of detection achievable.

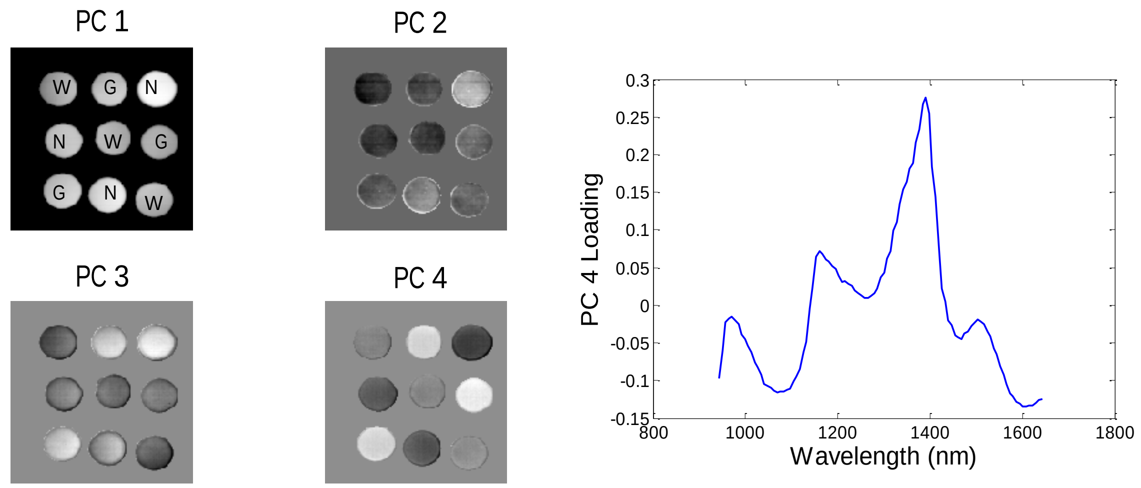

Figure 1 Principal component (PC) score images (left) and fourth PC loading plotted as a function of wavelength (right). Coding in the PC 1 score image indicates position of water (W), NaCl (N) and glucose (G) samples.

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MULTIVARIATE CURVE RESOLUTION AND ROTATION EVALUATION ON REMOTE SENSING HYPERSPECTRAL IMAGES

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MCR-ALS is applied to three different remote sensing hyperspectral images which were obtained by the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) operated by NASA and they are in public databases [1]. The first one is a reference image of Cuprite, Nevada, in 1997, which was with 224 spectral bands over 400-2500nm. The size of the data set is 614×512 pixels. The Cuprite area is arid with a small amount of vegetation cover, and has rock exposures comprising alteration zones characterized by the occurrence of key indicator minerals. The second image is from a remote sensing test site on the bay of San Francisco, a few kilometers north of the city of Mountain View, California. The site includes the Naval Air Station Moffet Field, agriculture fields, water ponds, salt banks, and man-made constructions such as several airplane hangars which today are museums. It is ideal for water variability, vegetation and urban studies. The third image is taken at the airport of the airfield in San Diego, California. It has size of 400×400, and it has 224 spectral bands over 400-2500nm. The study of this area includes vegetation, tarmac and concrete. Minerals in the first image, water, vegetation and urban in the second image and airplanes in the third image are investigated in the hyperspectral images. MCR-ALS is tested to analyze and resolve these areas with different characteristics. Results achieved show that MCR-ALS performs well for the resolution of these hyperspectral images from remote sensing. To check the extent of rotation ambiguities associated to a particular MCR solution under a set of constrains, MCR-BANDS [2, 3] was also applied to these datasets and to a dataset which was simulated using three spectral signatures extracted from the 1997 USGS Digital Spectral Library. The maximum and minimum of the relative signal contribution of each resolved pure component together with their corresponding spectra were estimated and their distribution maps (images) compared. . The obtained results confirm that MCR-BANDS results did include those profiles resolved by MCR-ALS and also by some other spectroscopic image analysis methods like VCA [4] and MVSA [5]).

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CHARACTERIZATION OF PLASTICS WITH HYPERSPECTRAL METHODS

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Plastic represents one of the larger categories among solid wastes. This depends on the fact that this material is continuously replacing some other one in many types of applications.

Plastic solid waste can be recycled to produce secondary raw materials. This allows decreasing the use of raw material and reducing the accumulation of material in landfill. For these reasons recycling represents an issue of remarkable economical and social importance [4].

Technologies for plastic recycling have to guarantee high-quality secondary raw material, complying with specific standards, for use in industrial applications. The market value of recycled plastics is considerably affected by the purity, degree of decontamination and homogeneity of the plastics [3].

Recycling may be accomplished via mechanical methods that usually involve the following steps: contaminant separation (plastics are separated from other types of materials such as paper or metal), separation of different types of plastic polymers (separated by flotation, density difference, aerodynamic or electrostatic properties, etc), washing and drying, shredding, comminution, agglutination, extrusion [1].

The separation step may be challenging due to the similarities in physical properties between several types of plastic materials [2]. Hyperspectral systems represent an interesting alternative to classical technologies to separate contaminants from plastic wastes and different types of plastic polymers. Those systems present low cost compared to other systems available on the market, high spectral resolution, high spatial and temporal resolution and significant rapidity.

In this study, we present an effective methodology for material classification that is particularly suitable for plastic materials. This methodology is based on the use of an innovative experimental device for acquiring and analyzing hyperspectral images. The device employs two ImSpector spectrometers; one spectrometer is centered in the visible range of the electromagnetic spectrum (400–1,000 nm), and the other device is centered in the near-infrared region (900–1,800 nm). Each imaging spectrograph is combined with an appropriate monochrome matrix camera equipped with an objective lens to form a spectral imaging device. This system simultaneously acquires the spectra of a line. Multiple images must be acquired to reconstruct a two-dimensional scene based on the combination of several lines.

The plastic materials analyzed belong to the types PET, PVC, PS, resins, LDPE and differ in color and density. Those materials have been placed on different supports in order to assess the spectral signature in different conditions. A spectroradiometer Fieldspec, manufactured by Analytical Spectral Devices - Inc. (Boulder, CO, USA), which operates in the range of wavelengths between 350-2500 nm complements the hyperspectral signature database.

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SOME COMMENTS ON THE CLASSIFIATION OF HYERSPECTRAL IMAGES

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Classification in general, and classiication of hyperspectral images in particular, can be operated in many different ways: there are different methods to choose among, and, once the method is chosen, several options or parameters to tune. Eventually, all the choices have an effect on the quality of the final model. In this communication, some relevant topics for the selection of an optimal classifier for hyperspectral images will be discussed in detail. In particular, attention will be focused on the distinction between a modeling and a discriminant approach and, in the latter case, on the comparison between a multi-class implementation (PLS2-DA) and the application of multiple "one against the rest" classifiers (PLS1-DA). Additionally, some comments on the selection of the pixels to be used as training and test sets will be made.

MULTI-TECHNIQUE IMAGE FUSION AND MULTIVARIATE CURVE RESOLUTION CONSIDERATIONS

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Every analytical imaging method has its own sensitivities and interferences. The ability to use multiple analytical techniques to analyze a single sample provides a chance to improve interpretation through improved specificity to chemical and physical variations in the sample. However, joining or „fusing" the multiple blocks of image data and analyzing that joined data involves a number of key decisions like how the individual image sets are scaled and preprocessed, how they are aligned spatially, and what numerical methods are used once the blocks are combined blocks are analyzed. In some cases, the decisions aren't critical and the same conclusions would be reached over a wide range of analysis conditions. In other cases, particularly when the analytical methods are very different in sensitivity, decisions can have a notable effect.

In this presentation, we will discuss the results of several fused image sets from samples we've been investigating using Raman, X-ray fluorescence, and laser-induced fluorescence. We will discuss how the various decisions were made and demonstrate the sensitivity to these decisions.

In addition, we will discuss the role that curve resolution constraints play in the analysis of fused image data sets. In previous work, we have seen that complex data sets can lead to difficult-to-interpret curve resolution results, but that using some simple algorithmic changes[1] can lead to more interpretable results. We will discuss the impact these methods have on curve resolution of fused images.

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IMAGE SAMPLING AND DECISION TREES – OPTIMIZATION OF HYPERSPECTRAL IMAGE CALIBRATION MODELS

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