Novel possibilities for industrial solutions through chemical colour imaging - A bridging of spectroscopy and industrial image processing

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Introduction

This work summarises the development, application and validation of an EC3^a system, and describes the configuration process for specific chemical properties, monitoring and classification of chemical images. An EC3 system encapsulates a high-speed hyperspectral imaging (HSI) camera paired with a data processing unit based on FPGA^b technology. Therefore, spectral image acquisition and spectral pre-processing, as well as feature extraction and feature processing, can be achieved in real-time. By applying chemometric models, the rather complex spectral information content of each spatial position observed is reduced to a distinct set of chemical information (object features). The transformation of this feature set into a chemical colour image (CCI) opens the possibility for processing spatial 2D-resolved molecular object information with well-introduced standardised image processing methods.

Hyperspectral imaging and image processing in the industrial field

Both spectroscopy and image processing are powerful disciplines with great applicability for today's industrial solutions.^{1,2} While spectroscopy allows measurement of specific information from molecular structure, image processing methods primarily deal with information based on brightness or colour and geometrical (spatial) information of objects. Combining both technologies introduces numerous possibilities for industrial solutions. During recent years HSI systems have become more important for industrial purposes.

Experience gained from working with HSI systems^{3,4} in industry has shown several limitations of this technology and numerous customer needs have been recognised. The biggest challenge of working with hyperspectral data in the industrial field is the large volume of data acquired and the complex nature of the data scanned.

The HELIOS NIR^c system of EVK^d gives an impression of the total data load. Since the system has been developed to be limited only by the sensor readout speed, data volumes to be processed are bigger than 400MBit.s⁻¹. Due to the additional data dimension in the spectral direction of almost a few hundred wavelength positions, the data volume appears to be poor regarding the spatial resolution capabilities but huge in terms of data load per second. Especially when bulk sorting, the resulting spatial resolution (along transport direction and lateral to transport direction) barely meets expectations for most applications. The demand for hyperspectral imaging solutions has increased in recent years. Therefore it is reasonable to assume that much faster sensors will be standard in the future. Processing sensory data on contemporary PC systems is quite challenging. For future sensors with further increased resolution new processing strategies must be found. Also, in the rough industrial environment the transfer of the data from the camera might restrict several applications in the future.

In addition to these hardware details, data processing and interpretation of hyperspectral data are complicated and time-consuming. Altogether, analysing a system using hyperspectral imaging needs a lot of time and expert knowledge. In terms of an in-line application these features are a problem. Compared to well-established image processing systems, the spectral information in the NIR is complex and not illustrative for non-experts. The interaction of maintenance or operational employees with the sensor system is therefore very restricted and in most cases not useful.

Besides these technical limitations, the acceptance of hyperspectral imaging to machine builders is diminished by an additional fact: these companies want to gain their own application know-how and want to

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^a Result of the technology project EC3: <u>EVK Chemical Colour Camera</u>

^b Field Programmable Gate Array

[°] Hyperspectral imaging camera system for the near infrared (NIR)

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define a unique selling proposition from this knowledge. This basic economic requirement is restricted by the necessity of continuous cooperation with the sensor supplier.

The technology project EC3

The technology project called EC3 aimed to fulfil customer needs and to overcome known limitations of contemporary hyperspectral imaging applications. All functionality gained in this project should be based on the existing hyperspectral imaging camera system HELIOS of EVK. The resulting sensor system therefore was developed with respect to an in-line application in an industrial field.

The major goal of this work was to exploit the application of hyperspectral imaging systems by developing a simplified standard methodology for image processing. The work was based on the assumption that chemical information originally represented by spectra can be approximated by a strongly reduced set of material properties. Furthermore, the informational content in a property set per measurement point should be processed as relational information represented as colour information. For example, the relation of properties P1:P2:P3 = 3:2:1, where P1 = red, P2 = green and P3 = blue results in a brown colour. By processing data by colour, the processing of chemical properties by their relation is achieved. Respective variances of relational information should be established by defining a confidence space of chemical property relations, e.g. for classification. The spatial distribution information of property relation classes should enable the extraction of object properties, therefore enabling the decision related to the individual measurement object, e.g. sorting purposes.

Since the main users of such a system were intended to be spectroscopy and chemometrics non-experts, e.g. machine builders and image processors, the configuration work regarding a hyperspectral imaging system must be dramatically simplified. For this purpose some methods are described which try to reduce the complexity of working with hyperspectral data. The project was ended by validation of such an in-line camera system. The industrial sorting of blueberries is given as an example of this process.

Methods

Here methods for establishing a straightforward approach to the application of chemical colour imaging in industry are described. Since both investigated technologies – image processing and multivariate data processing⁶ – have previously been well-explained, this work focuses mainly on describing the possibilities for combination.

Previewing hyperspectral data cubes – Vis transformation

The ability to transform spectral content into reduced but interpretable information facilitates the analysis of hyperspectral data. Here an unsupervised previewing method is outlined which enables the interpretation of chemical information in a spectrum in the way used for colour camera technology. The method roughly estimates the spectral content by 3 values gained from folding the spectra by 3 different "filter functions". For each spectrum in a hyperspectral (HS) data cube, 3 values are calculated and represented as 3 individual matrices of size S × T (S = number of sample points along spatial domain, T = number of sample points along time domain). Before the assignment to the colour channels of a RGB image, the matrices are scaled relative to their maximum and minimum value to the range of the output format (e.g. 0-255 for standard colour images).

Fig. 1 illustrates filter functions used and the result of this method applied to a HS data cube gained from measuring minerals of different categories. Before previewing, normalisation was applied to each spectrum in the cube. In Fig. 1 b) a lot of spectral details become "visible"; similar colours indicate spectra of similar spectral content and distinct colours indicate a distinct spectral content.



Figure 1. a) Filter functions used. b) Result of the previewing method for minerals of categories: talc (upper row), magnesite (middle row) and calcite (lower row). c) Normalised reflectance spectra at spatial location denoted by the + markers in b).

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Property extraction

In this section multivariate data processing methods are utilised in an illustrative way to allow non-experts of chemometrics to extract essential information from spectral datasets. The beginning of this work should be facilitated through the answering of 3 questions. By doing so, the user is guided though the configuration dependent on their task. Each configuration method results in a set of linear models to describe specific properties of the focused measurement objects.

The first question to be defined was: "What is the spectral content of the measurement objects?" For this purpose, principal component analysis⁵ (PCA) is applied to the selected spectra. The resulting loadings are applied to the HS data cube and result in a direct feedback showing the score images per principal component (PC). Because of the additional spatial information, these images are highly descriptive, allowing the user to explore the HS data cube regarding the variance information in selected spectra. Furthermore, if the analyses of chemically-different objects do not result in differences, other pre-processing methods might be necessary.

In terms of measuring the similarity to defined objects (or locations on objects), partial least square (PLS) calibration⁵ is used. This method is introduced by the question: "Is it necessary to constrain colours to represent certain chemical characteristics?" Spectra of marked locations are calibrated to a chosen colour. The colours for all other spectra in the HS data cube are predicted and immediately visualised. The user can do a quick validation by comparing their expectations to the resulting colour image. Each colour channel is separately calibrated. Therefore, 3 PLS-1 calibration algorithms are used to allow prediction of the individual colour channels. To prevent calibration on spectrally identical objects, the warning in this question should make the user verify the presence of spectral differences by doing a PCA first.



Figure 2. a) HS-Preview of polymers of category "PS" and "PVC", blue coloured regions show the influence of water. b) Property-scores gained from PCA. c) Given colours of method "constrain colours" (green and red regions). d) Predicted colours of method "constrain colours".

The property scores shown in Figure 2 b) illustrate the spectral variances in the data; PC1 separates the categories and PC3 corresponds to water (shown in Figure 2 a)). Figure 2 d) summarises similarities to calibrated spectra at locations shown in Figure 2 c); objects of category "PVC" are shown in green colour. The similarity to the common spectral information of the given spectra (Figure 2 c)) is rather different from object to object but reasonably constant within an object. This can be explained by a rather constant chemical composition in the objects but slight differences in the chemical composition from object to object.

The third question that can be answered is: "What is the proportion of ingredients?" As known from multivariate calibration the user has to specify given values for selected spectra. By using PLS a calibration model is calculated and applied to the HS data cube showing the prediction result as a spatially-resolved image.

Property relations - combining and scaling

As mentioned before, such a camera system exploits the combination of multivariate and image processing by combining chemical properties to relational information expressed as colour information. The combination of properties is done by the user by selecting 3 different linear models gained from property extraction. Before assigning the resulting property score matrices to the colour channels of a RGB image, each property score matrix has to be scaled to the value range of the RGB image (0-255 for standard colour images). Scaling can be done with respect to the value distribution of the property scores by applying the linear model to the HS data cube or by applying it to selected spectra. When scaling to the scores image of a HS data cube, surrounding objects might influence the scaling result (selected objects are not properly visualised). In case of scaling to the scores of selected spectra, unselected spectra of the same object might become over- or under-steered if their score value is out of the score value range of selected spectra.

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Processing of chemical colour images

Since the spatial 2D-resolved chemical relation information is represented by a standardised colour image format all capabilities of image processing can be exploited.¹ The transformation of the chemical RGB-information into the HSV-space⁶ (Hue, Saturation and Value or intensity) for example enables the separation of the colour impression (relation of chemical properties) from the intensity and therefore the absolute value of chemical properties. Furthermore, a decision per spatial object can be gained by applying object recognition⁷ algorithms and by evaluation of the spatial distribution of chemical information. Noisy information may be processed when applying image filtering techniques.⁸

Validation by industrial application of an EC3 system to sorting blueberries

During blueberry sorting, foreign materials like leaves, stems, bugs, stones, glass, metals and cap stems (stem rising from a fruit) have to be detected and separated.

System setup

Frozen blueberries (-15°C to -25°C) were sorted. The material was inspected in free fall processing, reflected light from the objects was collected along an illuminated line lateral to the falling direction. To be able to inspect the whole surface of objects, 2 HELIOS systems were used – one for inspection of the front and one for the backside. Table 1 summarises important instrumental parameters.

Table 1.	Key	parameters.
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2 I	
Spatial resolution (in falling direction)	2 mm (approx. 5 pixels in height for blueberries)
Spatial resolution (lateral to falling direction)	1.25 mm (approx. 8 pixels in width for blueberries)
Integration Time	2 ms
Spectral resolution	5 nm
Spectral range	1100 – 1500 nm
Sensor value range	0 – 4095 count (12 bit)
Pre-processing	First derivative, maximum normalisation
Background Treatment	When mean intensity < 180 count
Capacity of the sorting machine	Up to 1500 kg.hl ⁻¹ at 600 mm working width

Strategies for property extraction and relations

The configuration strategy of the EC3 system describes the material to be sorted by three properties: "Similar to blueberry", "wooden" and "Similar to bugs". In addition, NIR-inactive materials like glass should be separable from background through evaluation of the mean intensity reflected by parts compared to a stable "black" background. This functionality is provided by HELIOS by combining the colour information with the feature "mean intensity". Table 2 summarises the chemical colours.

Table 2. Chemical colour information versus object types.

Chemical colour information	Chemical property	Object type
Green	Similar to blueberry	Blueberry
Red	"wooden"	Stem, leaf, wooden parts
Blue	Similar to bug	Everything f bug-like chemical nature e.g fly, beetle.
Yellow-orange (e.g. brown)	Similar to blueberry and "wooden" in an undefined relation.	A blueberry with a wooden influence, e.g. attached stems or leafs.
Bluish-green, cyan	Similar to blueberry and bug in an undefined relation.	A blueberry and similar to bug.
Dark gray, black	Not similar or related to blueberry, "wooden" or bug.	All objects which do not have aforementioned properties, e.g. stones, glass, plastic, metal.
Pure white	From objects with reflected intensity beyond a certain limit.	Background

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Configuration of property extraction and relation

Sequences of a blueberry stream contaminated with stems, leaves and bugs were captured and visualised by the HS-previewing method. From the spatial representation and colour impression in the view, different object groups were recognised. Different spectral sets were taken from blueberries, isolated stems and leaves as well as bugs (pure objects). Applying PCA did not differentiate the objects – a configuration according to spectral variances was not possible because of the large noise content (caused by the short integration time and small objects) in the data. By means of the method "constrain colours" desired colours were assigned to the spectra of pure objects. As illustrated in Figure 3, spectra of blueberries and stems are not clearly distinct and noisy.



Figure 3. First derivative and normalised spectra of blueberry (blue) and stems (green and red) in the range $1.1-1.5 \mu m$. The lines represent the maximum of the value distribution per wavelength position. The shadows denote the σ -1 to σ -4 region per distribution.

Results

Objects were scanned and monitored in the chemical colour imaging format. Figure 4 gives an overview of the results.



Figure 4. Chemical colour image of a) blueberry, b) leaf, c) blueberry with attached leaf and d) thin metal wire.

As expected, the centres of blueberries were visualised in a pure green colour (not "wooden" and no similarity to bugs). At the borders, the green information decreases and some red information may appear (brownish colour in the first row of Figure 4 a)). This effect might be caused by reduced water information in the spectrum (decreased green – decreased blueberry similarity) and by increased "wooden" information (increased red) because of measurement of the skin. For experts in image processing, the detection of blueberries is simple because they always have a good portion of pixels in green. An example of the advantage of working with relational information is shown in Figure 4c). The rather small spectroscopic influence of a thin leaf attached to a blueberry means the chemical colour information at one end of the blueberry is in an indefinable state between pure red ("wooden") and green (blueberry). Image processing enables pixels of impure colour to be considered the combination of the contributing objects. Table 3 summarises the sorting accuracy for defined impurities. Each test was done with 30 pieces of each material group on the "free fall" sorting machine under real conditions.

Object	Quantity [%]	Reject Quantity [%]	Quality Quantity [%]
glass	100	100	0
wood	100	100	0
paper	100	100	0
plastic	100	96.67	3.33
insects	100	100	0
metal	100	100	0
BB	100	0	100
BB with CS>5mm	100	96.67	3.33
BB with AL>5mm	100	93.33	6.67

(BB = Blueberry; CS = Capstem; AL = Attached Leaf)

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Conclusion

The EC3 technology is bridging the gap between spectral imaging and imaging processing. Processing the large datasets produced by a HSI system was simplified by representing the spectral information in the CCI format. As a result, the scanned chemical information becomes immediately comprehensible for the user, is easier to understand for non-experts of spectroscopy and can be refined by image processing. By applying image processing to chemical information, the spatial distribution of the measurement results can also be taken into account. Besides the chemical information, this additional information enables new industrial solutions, especially when applying object-based image processing algorithms. The classification of objects according to their chemical properties is done by well-established colour classification methodology. Due to the large reduction of data achievable by chemical properties extraction, the transfer of data to PC systems is not restrictive. The configuration of hyperspectral imaging systems and handling of data has been opened to non-experts of spectroscopy and chemometrics.

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