Hyperspectral analysis of powder mixtures

Characterization of composition and distribution

Mixing of powders and granular materials is a critical step in many different industries including food, pharmaceutical, cosmetic, paper, plastic, and rubber industry. The selection of the optimal mixing procedure to achieve an even product quality is not straight forward. The mixing process will be affected by particle characteristics such as size, shape, density, and adhesion properties that may vary between different components in the same mix.

Good process and quality control requires an assessment of both product composition and homogeneity. This is traditionally done by random sampling and lab analysis. To achieve detailed information about the homogeneity of each batch, a high sample frequency is required. By using hyperspectral imaging, sample composition and distribution can be measured directly in the batch in real time covering a larger sample volume in a more time and cost-efficient manner. This also allows for the detection of impurities and their distribution within the powder.

In this example we will demonstrate how hyperspectral imaging can be used to measure the purity of a powder with 4 potential contaminants. The goal is to detect the purity of the base constituent independently of the type of contaminant. The data set was additionally used to show how hyperspectral imaging can be used to investigate sample homogeneity and to reveal poor mixing quality.

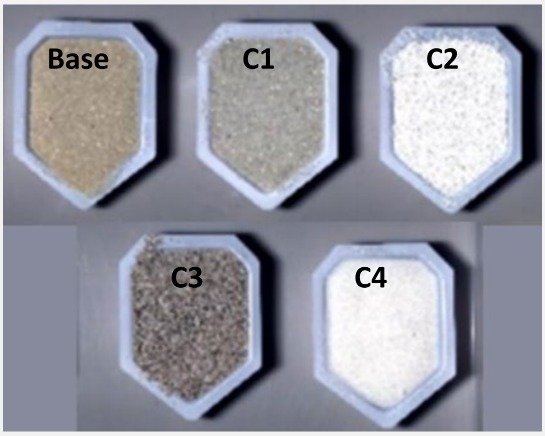
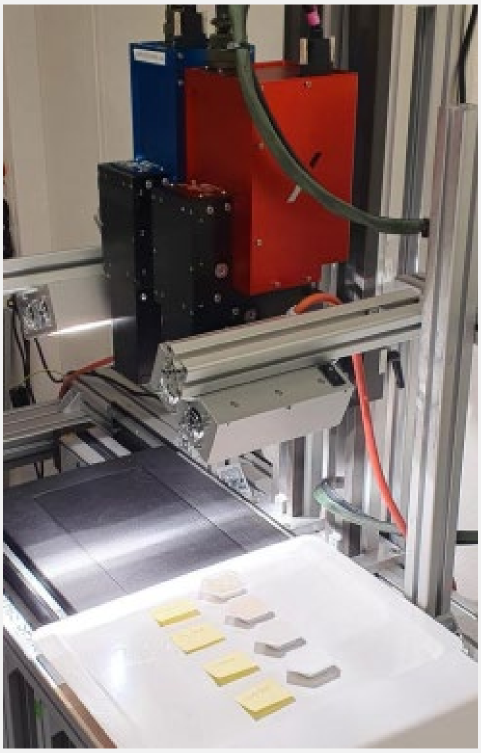


Figure 1. 5 different powders were investigated. One of the powders was used as the base for the experiment and the other 4 as contaminants (C1-C4). The contaminants were mixed with the base one at a time making up sample series of 16 samples for each contaminant with the concentrations of the contaminants ranging from 0.5 to 25 %. In addition to having different chemistry, the powders also differed in particle properties like size, shape density and adhesivity.

Figure 2. The samples were imaged in the laboratory with a HySpex Classic SWIR-384 camera (930-2500 nm) operating at a 30 cm distance. The camera has a spatial resolution of 250 µm and a spectral resolution of 5.45 nm.

The samples were scanned under the camera using a translation table. Two broadband halogen lamps were used as light sources. The acquired hyperspectral image data was analysed using the Breeze software, powered by Prediktera.

Quantification models were created using Partial Least Squares (PLS) regression validated with full cross validation. Models were built based on one contaminant at the time in addition to a global model including all samples.



The different powders all exhibit unique spectral properties in the SWIR range, even though some of the powders show similar absorption features (Figure 3). The base shows similar spectral properties as C4, and there is also a high similarity between sample C2 and C3. To achieve a good separation, a good spectral resolution is therefore required.

The spectral differences were sufficient to create quantification models with acceptable errors for all 5 powders. The model quality assessment was based on the correlation coefficient of cross validation (Q^2) and the Root Mean Square Error of Cross Validation (RMSECV). The models handling one contaminant at the time (Table 1) performed better than the global model (Table 2). The advantage with the global model is, however, that one can predict the content of base, and hence the purity, without knowing the nature of the contaminant.

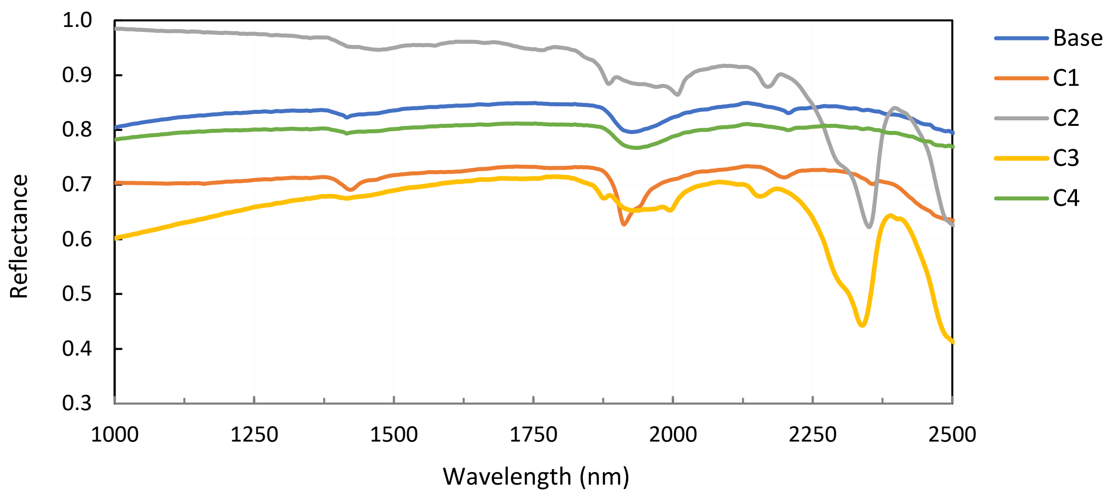


Figure 3. Average SWIR reflectance spectra of the 5 pure powders.

Table 1. PLS regression models for the base powder including different subsets of samples in the modelling.

Samples included in model	Q²	RMSECV	Principal Components
C1 – series	0.96	1.49	3
C2 - series	0.91	2.06	2
C3 - series	0.92	1.97	5
C4 - series	0.95	1.18	5
All samples	0.87	2.54	7

Table 2. PLS regression models for the different powders including all samples in the modelling (global model).

Powder type modelled	Q²	RMSECV
C1	0.95	1.12
C2	0.93	1.27
C3	0.89	1.63
C4	0.78	2.35
Base	0.87	2.54

The models can be used to predict the content of the different powder in each pixel. This gives an image of how well the powders have been mixed (Figure 4). To get a good overview of the homogeneity of the powder mix, a high spatial resolution is recommended to be as close as possible to separate between individual grains.

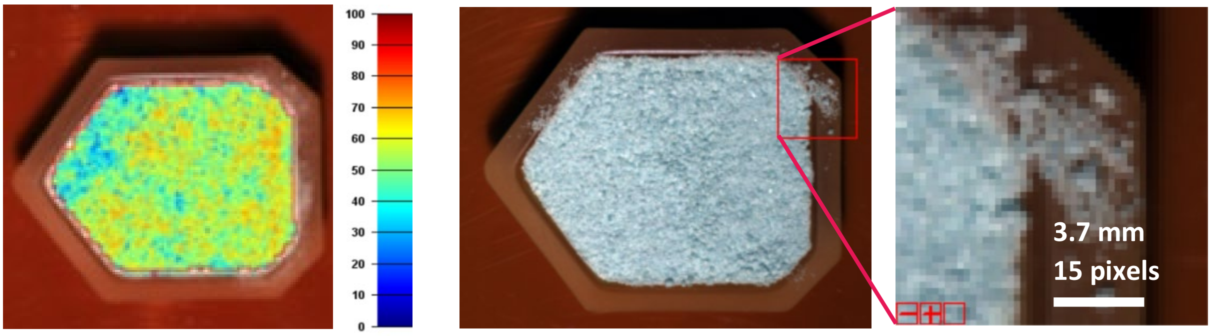


Figure 4. Left: Spatial distribution of base in a sample containing 75% base and 25% C2. The image is created by using the global PLS model to predict the base content in each pixel. Right: False color SWIR image of a pure base with an enlarged section showing the spatial resolution of the HySpex Classic SWIR camera.

This example shows that hyperspectral imaging can be used to predict the purity of powders without knowing the exact nature of the contaminant. Hyperspectral imaging can also be used to assess the mixing quality of powder mixtures given that the spatial resolution and the image quality is good. The HySpex cameras offer both superior spectral and spatial resolution with low smile and keystone effect**. Contact us to discuss your application and requirements with our specialists.

** Spectral and spatial misregistration. Visit www.hyspex.com for technical information on high-end hyperspectral cameras.

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