Abstract

Different quantitative tablet mapping methods in near infrared pushbroom hyperspectral imaging and their suitability for different sample sets

Timo Hyvärinen[1], Harri Karjalainen[1]* and Pekka Teppola[2]

[1]SPECIM, Spectral Imaging Ltd, Oulu, Finland
[2]Technical Research Centre of Finland, Kuopio, Finland
*Corresponding author: harri.karjalainen@specim.fi

Introduction

Hyperspectral imaging is being developed into a recognised and efficient chemical mapping method in the pharmaceutical industry. It is currently used in research laboratories and for formulation development and is now starting to penetrate into quality assurance and PAT applications. Several of these applications require Quantitative Mapping results. Chemometric methods to create calibration models with a minimal number of calibration samples were investigated with the aim of using only spectra of the pure components and one sample with known concentrations.

Materials and Methods

Several tablet sample sets with known average component concentrations were manufactured. The sample sets included products made of from three to six components. For each product, a large range of known concentration formulations were manufactured. The samples were imaged with a sisuCHEMA SWIR (970-2500 nm) push-broom hyperspectral imaging station. The spatial resolution was set to 30 µm in order to map the uniformity of the samples in detail. CLS, PLS-DA and SBC methods with a single calibration sample and pure spectra were compared to traditional PLS calibration with a large calibration sample set.

Results and Discussion

A PLS-DA calibration model based on a single calibration sample provided excellent quantitative results with an experimental 3-component product consisting of Ibuprofen, Lactose and MCC. PLS with multiple samples provided only a minor improvement in this case whereas PLS worked significantly better in quantitative mapping of a 6-component product and low concentrations than a single sample PLS-DA model. Here, the PLS-DA model provided a semi-quantitative map of the component distribution which is still valuable for rapid screening and trouble-shooting purposes. Additional experiments are being conducted to gain a wider understanding of the applicability of the methods and to see if the performance of a single sample calibration could be improved by adding one or two calibration samples while still keeping the calibration labour and cost drastically lower than in the traditional approach.

Conclusion

Single sample calibration methods, particularly PLS-DA, can provide excellent results for screening and trouble-shooting purposes. They also have potential for precise quantitative mapping of simple products.

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