

Abstract

Portable Raman, mid-infrared and near infrared spectrometers: the future of in-situ chemical quality control instrumentation?

Lars Herberholz, Sedakat Altinpinar, Damir Sorak and Heinz W. Siesler*

Department of Physical Chemistry, University of Duisburg-Essen, D 45117 Essen, Germany

*Corresponding author: hw.siesler@uni-due.de

Introduction

Recently, miniaturisation of Raman, mid-infrared (IR) and near-infrared (NIR) spectrometers has made substantial progress. While the mid-infrared systems are based on attenuated total reflectance (ATR) measurements, near-infrared spectrometers operate in the diffuse reflection or transmission mode. The reduction in instrument size, however, must not be accompanied by a reduction in measurement performance and miniaturisation will only have a real impact on chemical quality and process control if Raman and IR/NIR spectra of acceptable quality can be obtained with the portable instruments. Thus, for selected applications comparative studies between the different types of spectrometers and between conventional laboratory spectrometers are required in order to evaluate which is the best approach and whether these new instrumental developments can effectively replace laboratory systems.

Materials and Methods

Miniaturised Raman, IR and NIR spectrometers were applied in comparative performance tests between each other and with laboratory instruments for quantitative analyses of various quality control applications. Specifically, the results for a pharmaceutical drug formulation and hydrocarbon-contaminated soil will be reported.

Results and Discussion

For the pharmaceutical drug formulation containing three active ingredients the PLS calibration models based on spectra measured in diffuse reflection with the hand-held NIR spectrometer provided the best prediction performance relative to the other miniaturised instruments. Furthermore, it will be shown that the portable NIR spectrometer proved suitable for the qualitative and quantitative evaluation of different hydrocarbon contaminants in soil by in situ diffuse reflection measurements.

Conclusion

The presented results demonstrate that in the near future miniaturised spectrometers can – at least for in-the-field and in situ chemical quality control - substitute for conventional laboratory instruments.