Application Note AN-NIR-083

Quality Control of HDPE, LDPE, and PP

Non-destructive determination of polymers within one minute with NIRS

Identification of individual polymers with FT-IR spectroscopy can be a challenge due to sample inhomogeneity especially when larger sample sizes need to be analyzed.

This application note demonstrates that the DS2500 Solid Analyzer operating in the visible and near infrared spectral region (Vis-NIR) provides a **reliable and fast solution** for the identification of high-density polyethylene (HDPE), low-density polyethylene (LDPE), and polypropylene (PP). With **no sample preparation or chemicals needed**, Vis-NIR spectroscopy allows the identification of larger inhomogeneous sample amounts in **less than a minute**.

EXPERIMENTAL EQUIPMENT

HDPE, LDPE, and PP pellets were measured in reflection mode with a DS2500 Solid Analyzer over the full wavelength range (400–2500 nm). A rotating DS2500 Large Sample Cup was employed to overcome the distribution of varied particle sizes and chemical components. This allowed automated measurements at different sample locations for a reproducible spectrum acquisition. As displayed in Figure 1, samples were measured without any preparation. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.

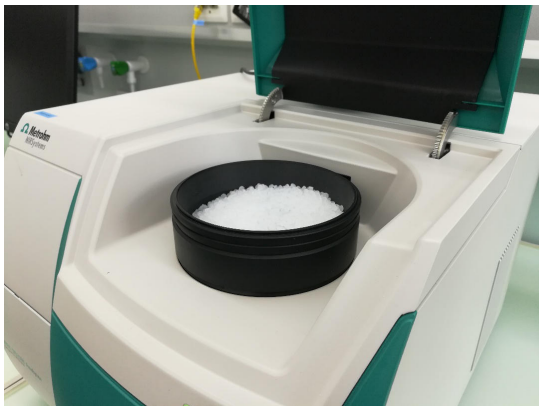

Figure 1. DS2500 Solid Analyzer and PE pellets present in the rotating DS2500 Large Sample Cup.

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
DS2500 Analyzer	2.922.0010
DS2500 Large Sample Cup	6.7402.050
Vision Air 2.0 Complete	6.6072.208

RESULT

A correlation algorithm was applied to the measured Vis-NIR spectra (Figure 2) to create a prediction model for the identification of the individual polymer types. The quality of the prediction was evaluated using built-in statistical tools, which display the correlation value distribution between Vis-NIR prediction and product class (Figure 3). The high correlation values of 0.985 and above, together with the fact that no polymer was misidentified, highlight the feasibility of NIR spectroscopy for identification of different polymer types.

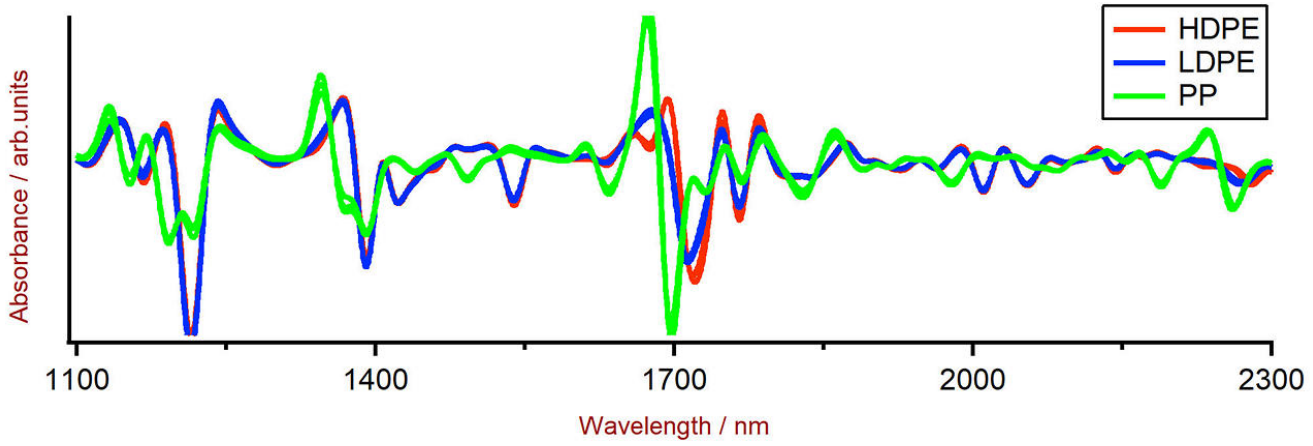

Figure 2. Selection of HDPE, LDPE, and PP NIR spectra (pre-treated with a 2nd derivative) obtained using a DS2500 Analyzer. Clear differences for the different polymer types are visible in the wavelength region around 1700 nm.

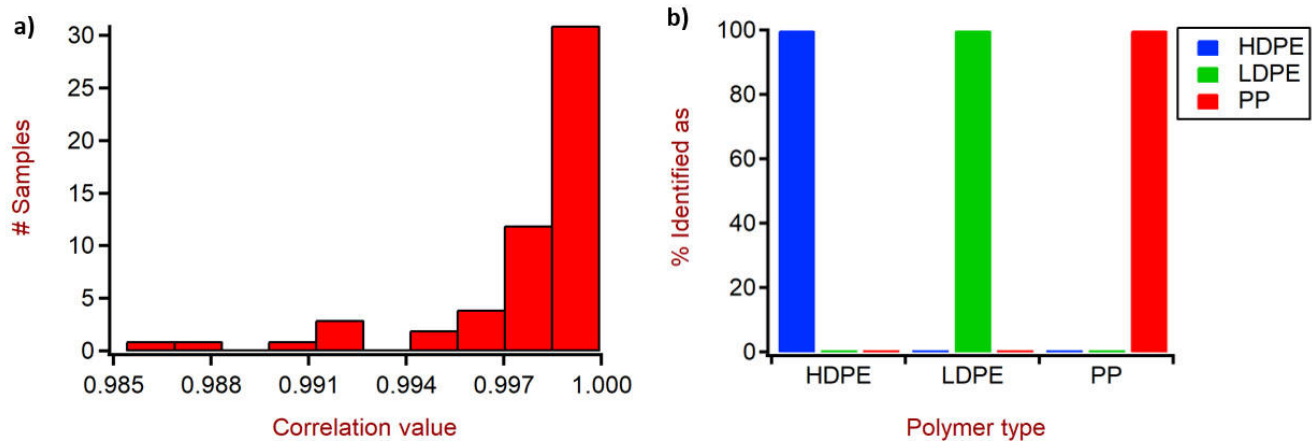

Figure 3. Correlation value histogram for the identification of the individual polymer types. (b) All polymer types in the sample set were identified correctly.

CONCLUSION

This application note demonstrates the feasibility of NIR spectroscopy to identify different types of polymers. In comparison to the FT-IR spectroscopy method, **no sample preparation is needed**. Further, the rotating sample cup system allows also the **fast analysis of large inhomogeneous sample sizes**.

CONTACT

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DS2500 Solid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Analyzer is the tried and tested, flexible solution for routine analysis of solids, creams, and optionally also liquids along the entire production chain. Its robust design makes the DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.

The DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The DS2500 Analyzer meets the demands of the pharmaceutical industry and supports users in their day-to-day routine tasks thanks to its simple operation.

Thanks to accessories tailored perfectly to the instrument, optimum results are achieved with every sample type, no matter how challenging it is, e.g. coarse-grained solids such as granulates or semi-solid samples such as creams. The MultiSample Cup can help improve productivity when measuring solids, as it enables automated measurements of series containing up to 9 samples.

DS2500 large sample cup

Large sample cup for the spectral recording of powders and granulates in reflection at various sample positions using the NIRS DS2500 Analyzer.

Vision Air 2.0 Complete

Vision Air - Universal spectroscopy software.

Vision Air Complete is a modern and simple-to-operate software solution for use in a regulated environment.

Overview of the advantages of Vision Air:

- Individual software applications with adapted user interfaces ensure intuitive and simple operation
- Simple creation and maintenance of operating procedures
- SQL database for secure and simple data management

The Vision Air Complete version (66072208) includes all applications for quality assurance using Vis-NIR spectroscopy:

- Application for instrument and data management
- Application for method development
- Application for routine analysis

Additional Vision Air Complete solutions:

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)