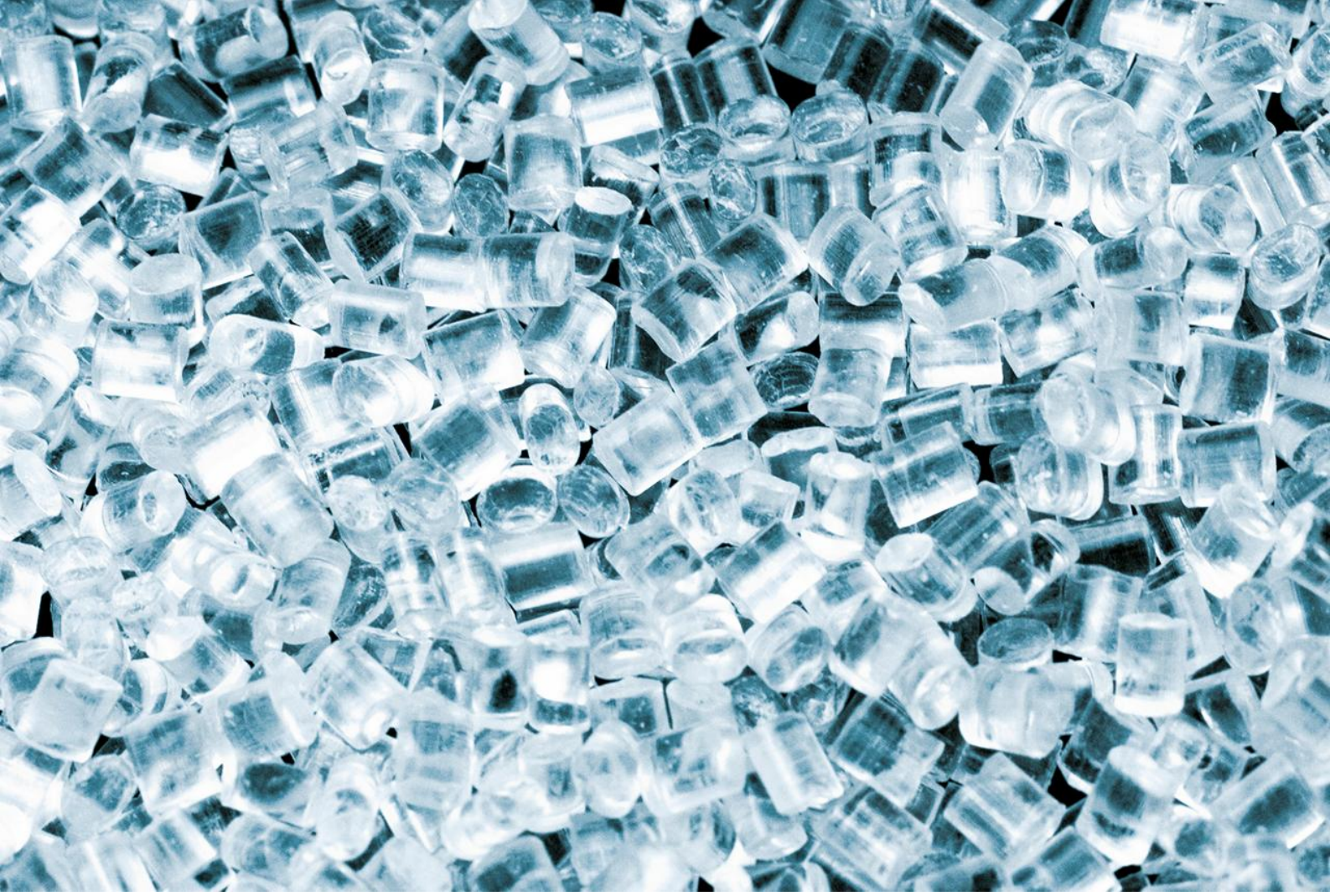

Application Note AN-NIR-081

Quality Control of Polyethylene

Reliable determination of PE density within one minute using NIRS

Determination of the density of polyethylene (PE) (ASTM D792) is normally a challenging procedure due to reproducibility difficulties. Since this parameter is most frequently used to determine the PE type, alternative methods which are sensitive to molecular structure such as FT-IR spectroscopy are also common. However, measurement via FT-IR can also be problematic when larger sample sizes must be analyzed due to sample inhomogeneity.

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 determination of the density of PE. With **no sample preparation or chemicals needed**, Vis-NIR spectroscopy allows the analysis of larger, inhomogeneous sample sizes of PE in **less than a minute**.

EXPERIMENTAL EQUIPMENT

PE pellets were measured in reflection mode over the full wavelength range (400–2500 nm) of the DS2500 Solid Analyzer. 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.

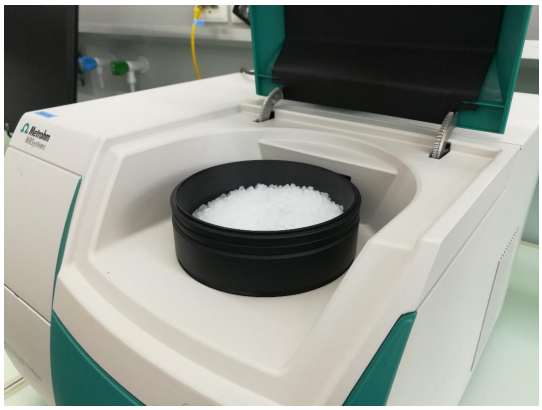

Figure 1. DS2500 Solid Analyzer and PE pellets present in the rotating DS2500 Large Sample Cup.

Table 1. Hardware and software equipment overview

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

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for quantification of the density content. The quality of the prediction models was evaluated using correlation diagrams, which display the relationship between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

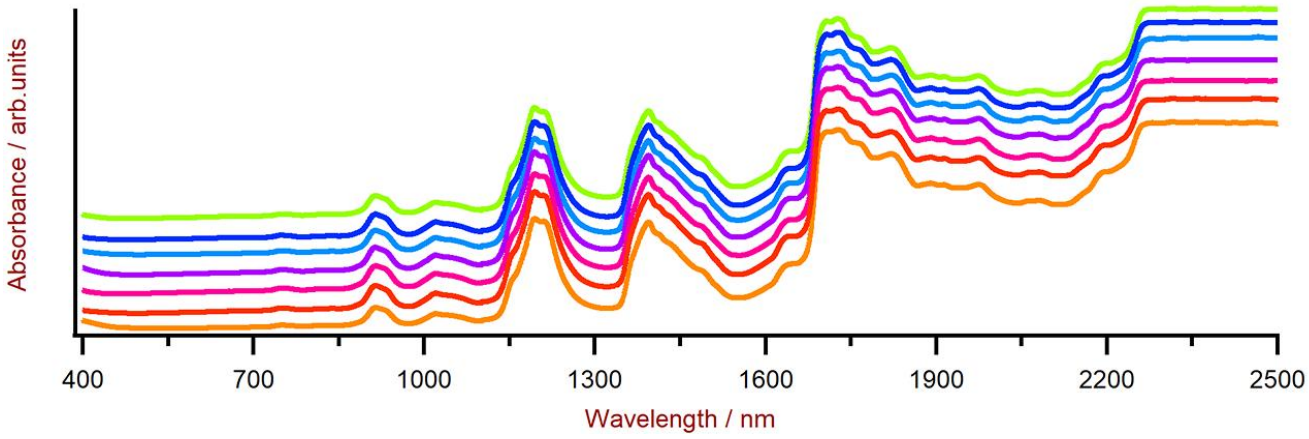

Figure 2. Selection of PE Vis-NIR spectra obtained using a DS2500 Analyzer and a rotating DS2500 Large Sample Cup. For display reasons a spectra offset was applied.

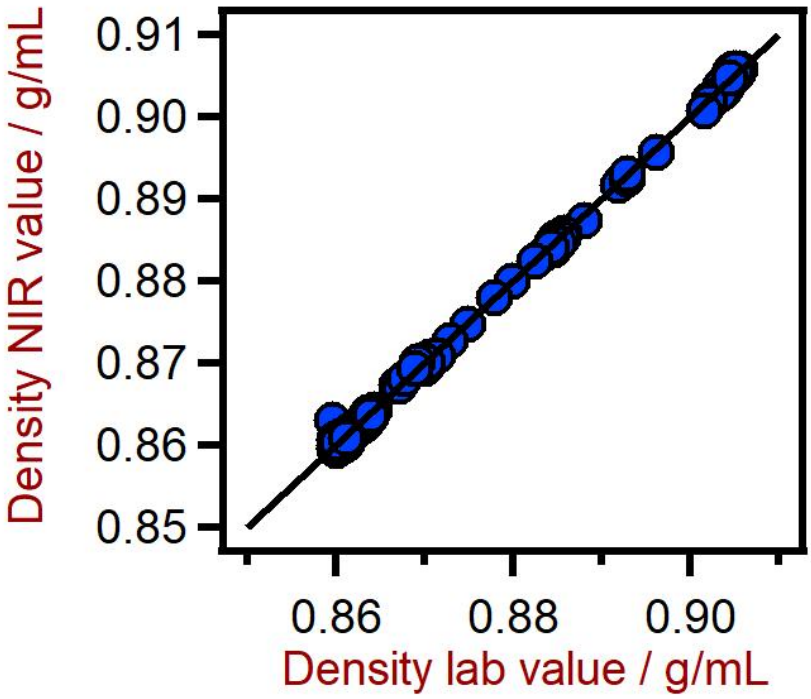

Figure 3. Correlation diagram for the prediction of the density of PE using a DS2500 Solid Analyzer. The density lab value was evaluated using densimetry.

Table 2. Figures of merit for the prediction of the density of PE using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.991
Standard error of calibration	0.0005 g/mL
Standard error of cross-validation	0.0005 g/mL

CONCLUSION

This application note demonstrates that the density of PE can be determined easily with NIR spectroscopy. Since no sample preparation is needed, samples are analyzed as they are, which allows for simple operation leading to highly precise results (0.0005 g/mL, see Table 2).

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