



Application Note AN-NIR-081

聚乙的量控

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.

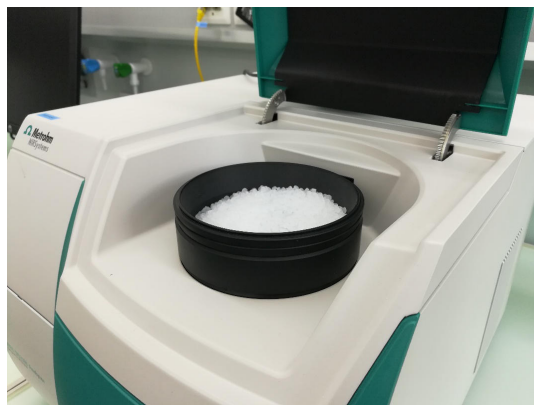


Figure 1. DS2500 Solid Analyzer and PE pellets present in the rotating DS2500 Large Sample Cup.

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.

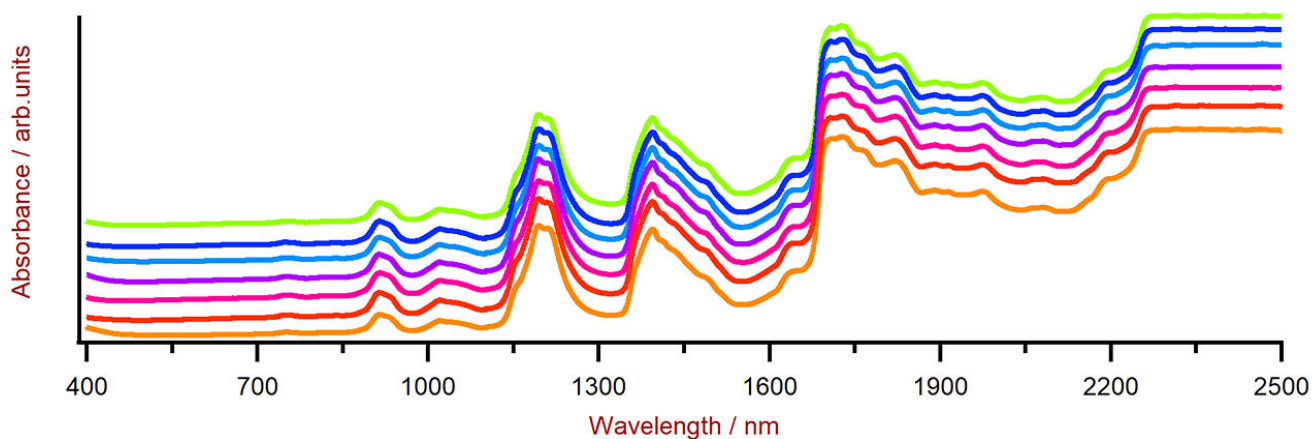


Figure 2. Selection of PE Vis-NIR spectra obtained using a DS2500 Analyzer and a rotating DS2500 Large Sample Cup. For display reasons a spectra offset was applied.

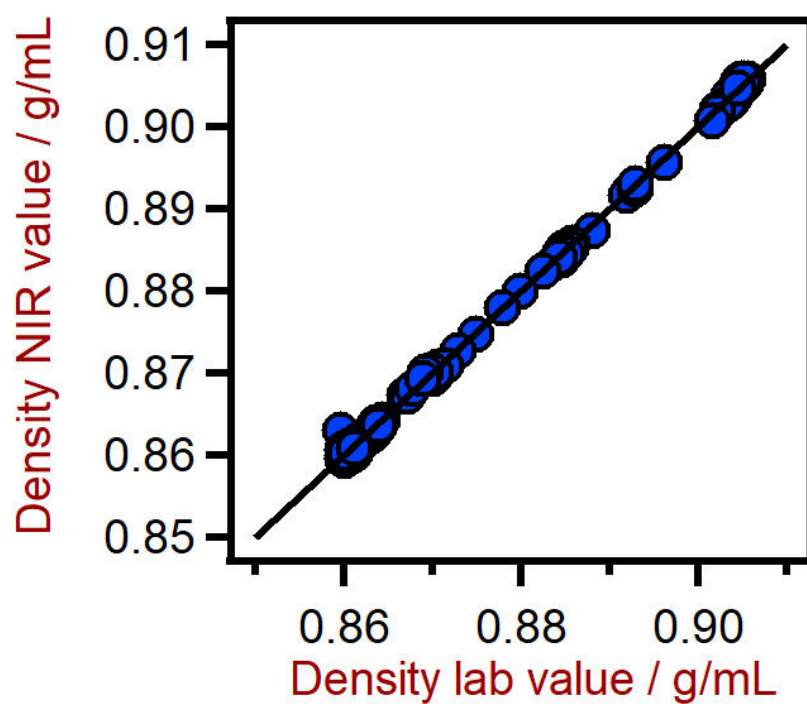


Figure 3. Correlation diagram for the prediction of the density of PE using a DS2500 Solid Analyzer. The density lab value was evaluated using densimetry.

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**).

CONTACT

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DS2500 Solid Analyzer

固的近外光,用于生境和室中的量。

DS2500 分析是的活解决方案,用于整个生程中的固体、乳膏和液体行常分析。其固的使 DS2500 Analyzer 分析不受灰、湿度、振和温度波的影,因此非常用于在劣的生境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光范,并能在不到一分内提供准和可再的果。DS2500 Analyzer 足制行的要求,并由于操作便而能助用完成其日常工作任。

由于与匹配,附件可以承受任何具有挑性的品型,例如:粒料之的粗粒固体或乳膏之的半固体品,可得果。量固体的候,使用 MultiSample Cup 可以提高生率,可以自批量量多 9 个品。



Vision Air 2.0 Complete

Vision Air – 通用的光分析件。

Vision Air Complete 是用于管范境的先易用的件解决方案。

Vision Air 点一:

- 便捷的件用和配的用界面保了直的操作方式
- 操作程的建与方式
- SQL 数据,可安全且地管理数据

Vision Air Complete (66072208) 版本包含所有用于可近外光分析量保程的用:

- 器和数据管理用
- 方法用
- 常分析用

其它 Vision Air Complete 解决方案:

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



DS2500

用于在不同品位置使用 NIRS DS2500 Analyzer 采集粉末和粒反射光的大号品容器。