



Application Note AN-NIR-081

聚乙烯的质量监控

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.

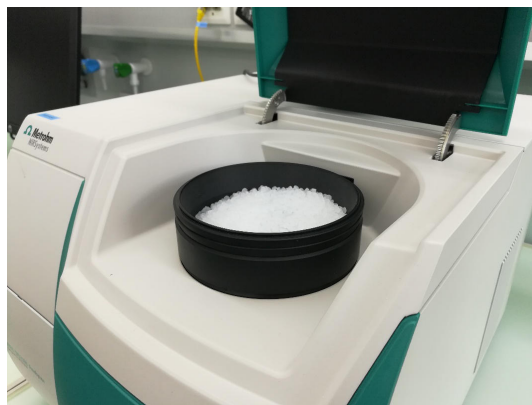


Figure 1. DS2500 Solid Analyzer and PE pellets present in the rotating DS2500 Large Sample Cup.

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.

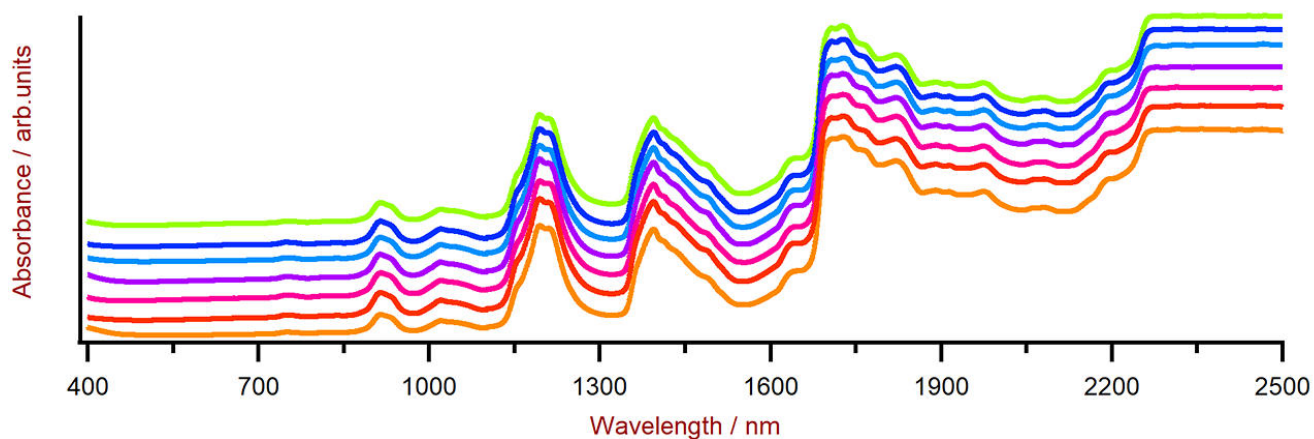


Figure 2. Selection of PE Vis-NIR spectra obtained using a DS2500 Analyzer and a rotating DS2500 Large Sample Cup. For display reasons a spectra offset was applied.

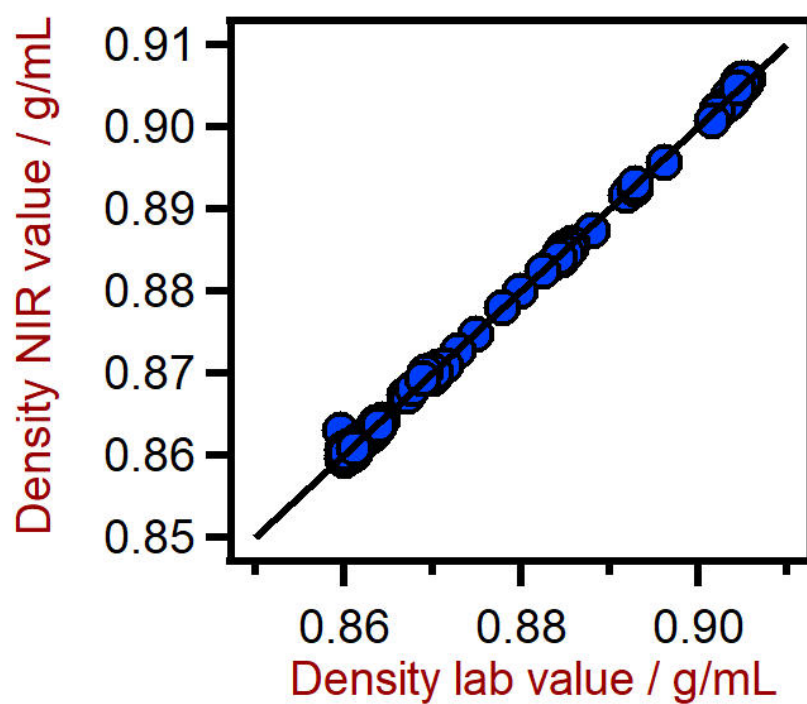


Figure 3. Correlation diagram for the prediction of the density of PE using a DS2500 Solid Analyzer. The density lab value was evaluated using densimetry.

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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 分析仪是经过验证的灵活解决方案,用于对整个生产链过程中的固体、乳膏和液体进行常规分析。其坚固结实的设计使 DS2500 Analyzer 分析仪不受灰尘、湿度、振动和温度波动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光谱范围,并能在不到一分钟时间内提供准确和可再现的结果。

DS2500 Analyzer 满足制药行业的要求,并由于操作简便而能帮助用户完成其日常工作任务。

由于与设备匹配,附件可以承受任何具有挑战性的样品类型,例如:粒料之类的粗颗粒固体或乳膏之类的半固体样品,可获得结果。测量固体的时候,使用 MultiSample Cup 可以提高生产率,可以自动批量测量多 9 个样品。



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
- 常规分析应用

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

用于在不同样品位置处使用 NIRS DS2500 Analyzer 采集粉末和颗粒反射光谱的大号样品容器。