



Application Note AN-NIR-083

高密度聚乙烯(HDPE)、低密度聚乙烯(LDPE)和聚丙烯(PP)的质量控制

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.

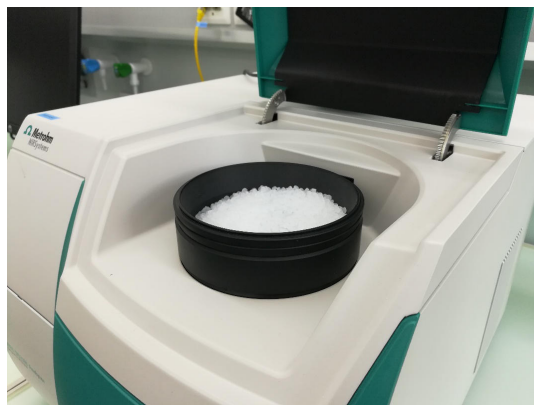


Figure 1. DS2500 Solid Analyzer and PE pellets present in the rotating DS2500 Large Sample Cup.

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.

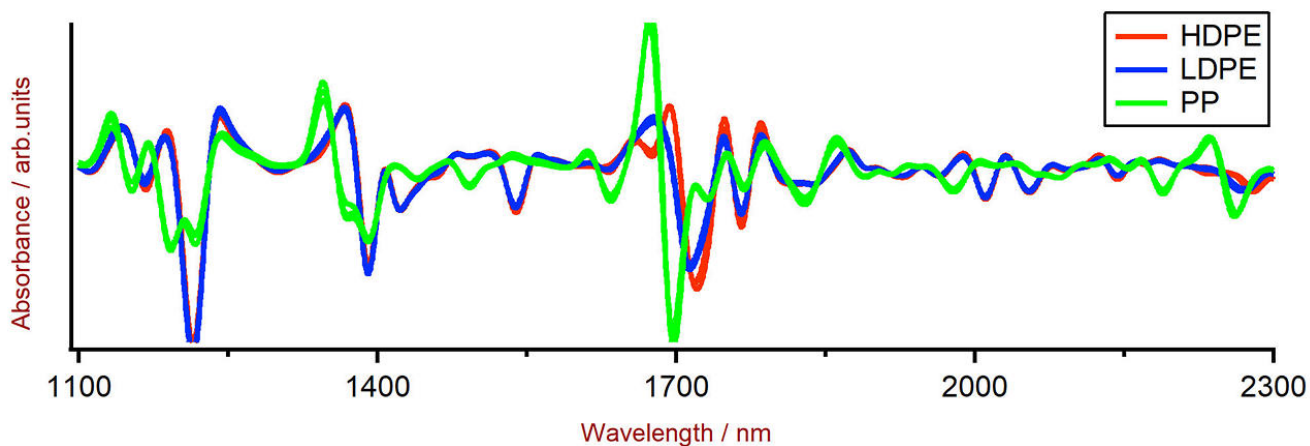


Figure 2. Selection of HDPE, LDPE, and PP NIR spectra (pre-treated with a 2nd derivative) obtained using a DS2500 Analyzer. Clear differences for the different polymer types are visible in the wavelength region around 1700 nm.

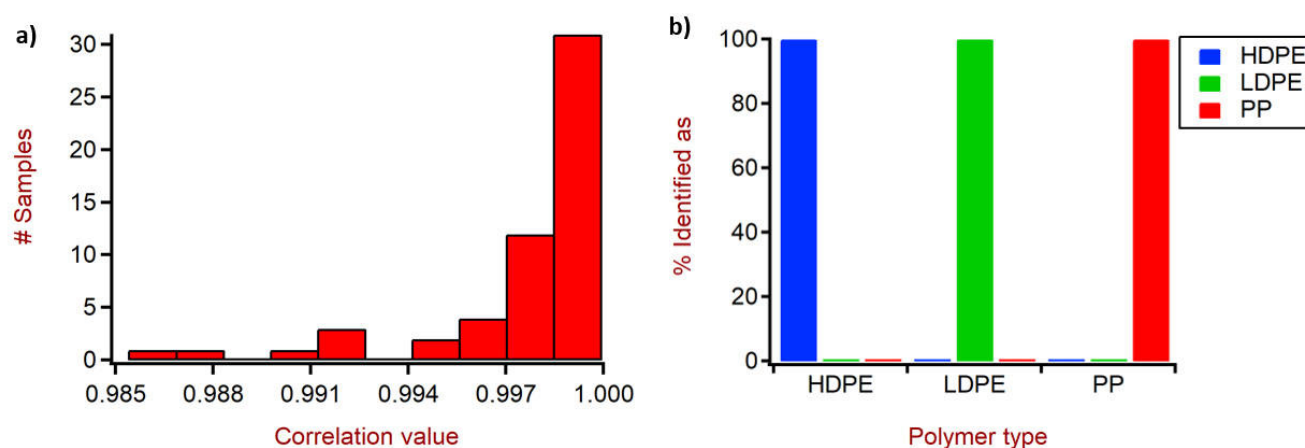


Figure 3. Correlation value histogram for the identification of the individual polymer types. (b) All polymer types in the sample set were identified correctly.

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.

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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。



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。



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)