



Application Note AN-NIR-098

PVC 粒料的质量控制

Determine molecular weight easily within seconds

PVC (polyvinyl chloride) has unique properties when compared to other olefin-derived plastics that only contain carbon and hydrogen atoms in their chemical structure. Some PVC features include increased chemical and mechanical stability as well as fire retardant properties. The molecular weight of the polymer has a significant influence on these properties. Molecular weight is defined here as the average weight of the molecules that make up a polymer, and this value gives an indication of the length of the polymer chains. To monitor the

PVC quality, it is important to measure the molecular weight during the production process. The standard method to determine PVC molecular weight is by size exclusion chromatography (SEC). This analytical method is time-intensive and requires trained personnel to perform.

Determining the molecular weight of PVC is easier with near-infrared spectroscopy (NIRS). NIRS provides results in **just a few seconds** and can quickly indicate when adjustments to the production process are necessary.

EXPERIMENTAL EQUIPMENT

33 PVC samples with varying molecular weights from 113000–192000 g/mol were measured on the DS2500 Solid Analyzer. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.



Figure 1. DS2500 Solid Analyzer

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
NIRS DS2500 Solid Analyzer	2.922.0010
Vision Air 2.0 Complete	6.6072.208
NIRS large sample cup	6.7402.050

RESULT

All 33 measured Vis-NIR spectra (**Figure 2**) were used to create a prediction model for quantification of molecular weight. The quality of the prediction model was evaluated using the cross-validation algorithm which displays a very

high correlation between Vis-NIR prediction and the reference values. The respective figures of merit (FOM) display the expected precision of a NIRS prediction during routine analysis (**Table 2**).



Figure 2. Vis-NIR spectra of PVC granulate samples with different molecular weights measured on a DS2500 Solid Analyzer.



Figure 3. Correlation diagram for the prediction of PVC molecular weight using a DS2500 Solid Analyzer.

Table 2. Figures of merit for the prediction of the molecular weight of PVC granulate samples using a DS2500 Solid Analyzer.

Figures of merit	Value
R^2	0.988
Standard error of calibration	3640 g/mol
Standard error of cross-validation	5375 g/mol

CONCLUSION

This application note demonstrates the feasibility to determine the molecular weight in PVC granulate samples with NIR spectroscopy. The PVC molecular weight was successfully determined with NIRS only differing from the

reference data with an average of 1.5%. Vis-NIR spectroscopy enables a fast determination with no sample preparation and has proven itself as a suitable method to measure PVC molecular weight.

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。