Application Note AN-NIR-098

Quality Control of PVC granulate

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 providesresultsin 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).

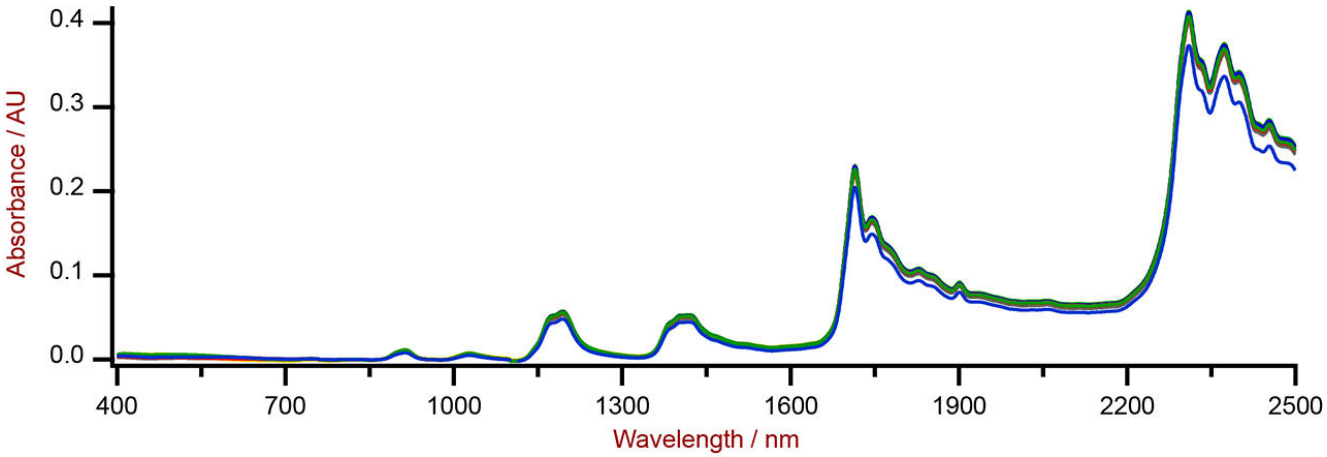

Figure 2. Vis-NIR spectra of PVC granulate samples with different molecular weights measured on a DS2500 Solid Analyzer.

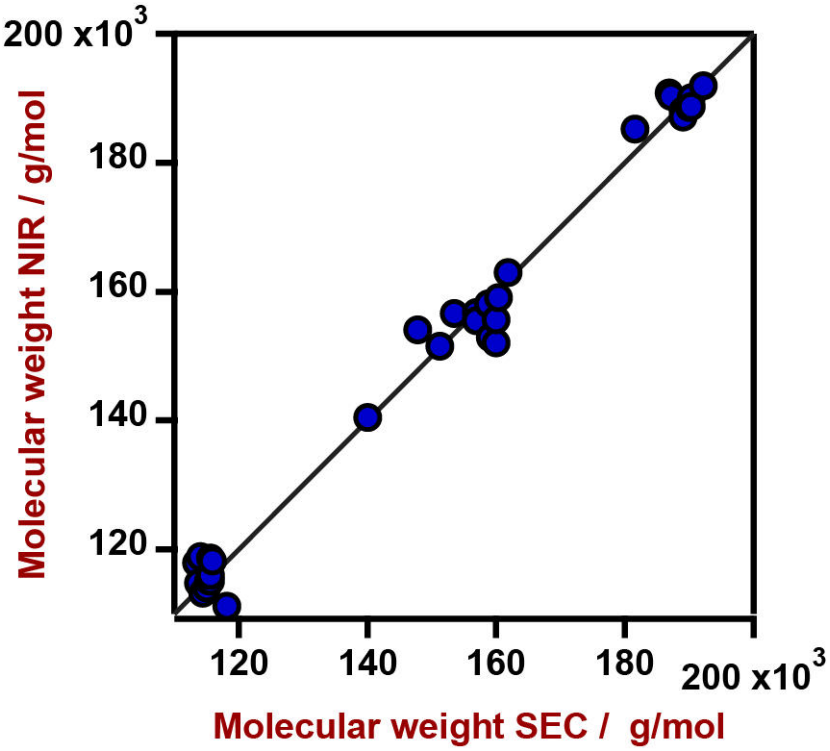

Figure 3. Correlation diagram for the prediction of PVC molecular weight using a DS2500 Solid Analyzer.

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.

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