



Application Note AN-NIR-024

# Quality control of pyrolysis gasoline

## Determination of diene value within one minute using NIRS

Pyrolysis gasoline (Pygas) is a byproduct of ethylene production, which contains unwanted conjugated diolefins making it unsuitable as a motor fuel. To overcome this limitation, the olefin content needs to be reduced below 2 mg/g pygas in a selective hydrogenation unit (SHU). The diene value, or maleic anhydride value (MAV), is usually determined by the

Diels-Alder wet chemical method (UOP326-17).

This wet chemical method requires several hours to perform by highly trained analysts. In contrast to the primary method, near-infrared spectroscopy (NIRS) is a cost-efficient and fast analytic solution for the determination of diene value in pyrolysis gasoline.

## EXPERIMENTAL EQUIPMENT

99 pygas samples were analyzed on a NIRS XDS RapidLiquid Analyzer equipped with 8 mm disposable glass vials. All measurements were performed in transmission mode from 400 nm to 2500 nm. The temperature control was set to 40 °C, to provide a stable sample environment. For convenience reasons disposable vials with a path length of 8 mm were used, which made a cleaning procedure obsolete. The Metrohm software package Vision Air Complete was used for data acquisition and prediction model development.



**Figure 1.** Samples filled in disposable vials with 8 mm path length.

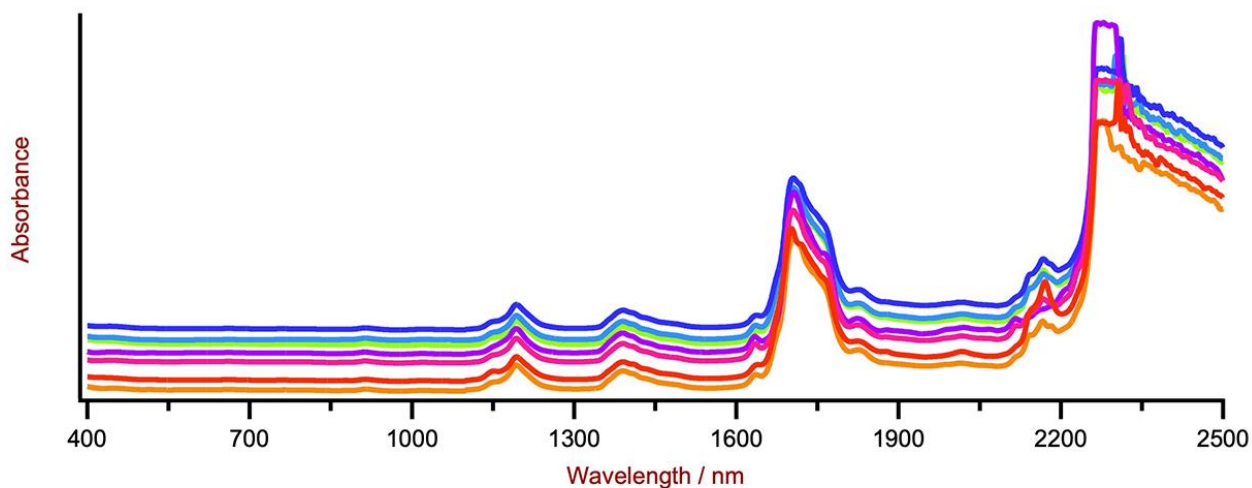
**Table 1.** Hardware and software equipment overview

Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208

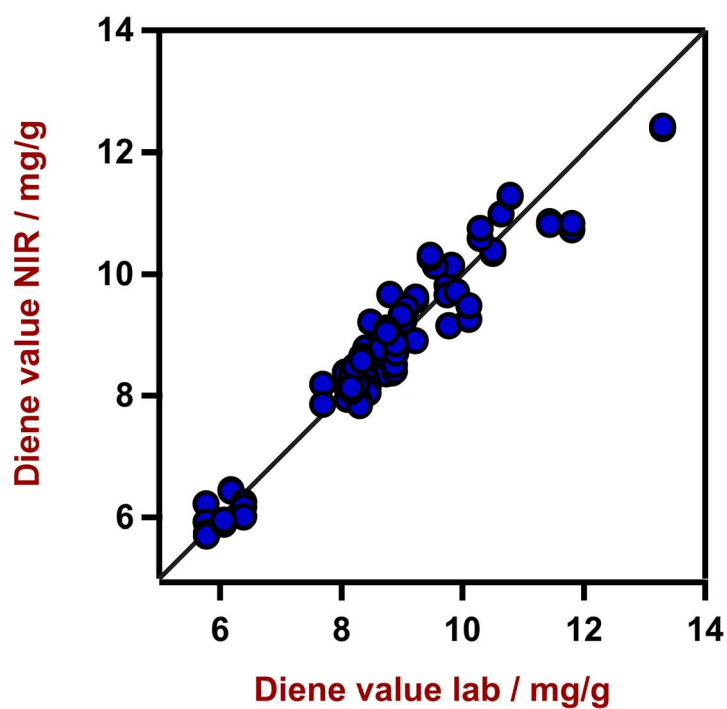
## RESULT

The obtained Vis-NIR spectra (**Figure 2**) were used to create a prediction model for the diene value determination. To verify the quality of the prediction model, correlation diagrams were created which

display the correlation between Vis-NIR prediction and primary method values (**Figure 3**). The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.



**Figure 2.** Selection of pyrolysis gasoline Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and 8 mm disposable vials. For display reasons a spectra offset was applied.



**Figure 3.** Correlation diagram for the prediction of the diene value using a XDS RapidLiquid Analyzer. The lab values were determined according to the UOP326-17 method.

**Table 2.** Figures of merit for the prediction of the diene value using a XDS RapidLiquid Analyzer.

Figures of merit	Value
$R^2$	0.9253
Standard error of calibration	0.42 mg/g
Standard error of cross-validation	0.46 mg/g

## CONCLUSION

This application note shows the feasibility of NIR spectroscopy for the analysis of diene value in pyrolysis gasoline. In comparison to the wet chemical

method UOP326-17 (**Table 3**), the time to result is a major advantage of NIR spectroscopy, since a single measurement is performed within one minute.

**Table 3.** Time to result with conventional UOP-326 wet chemistry analysis

Parameter	Method	Time to result and workflow
Diene value	Diels Alder (UOP326-17)	6 hr; reflux, hydrolysis, titration

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