



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.

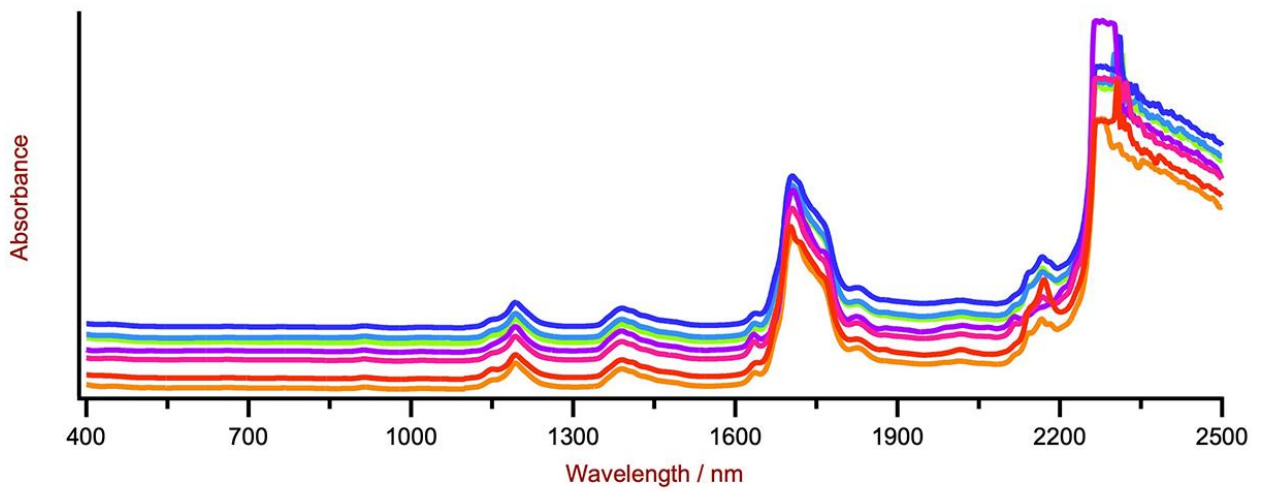
**Table 1.** Hardware and software equipment overview

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

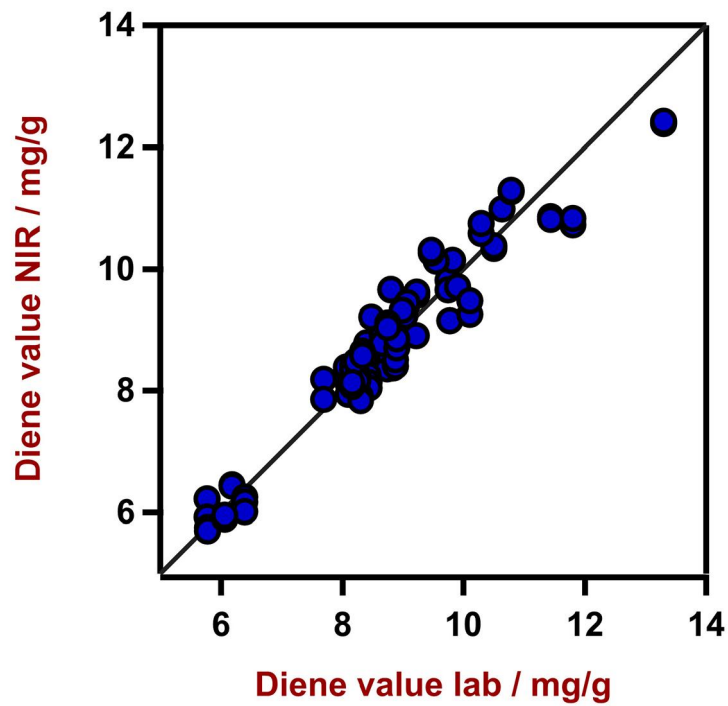
## RESULT

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 <sup>2</sup>	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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### NIRS XDS RapidLiquid Analyzer

Des analyses rapides et précises de liquides et suspensions de toutes sortes.

L'analyseur NIRS XDS RapidLiquid Analyzer permet des analyses rapides et précises de formules et substances liquides. Des résultats de mesure précis obtenus par simple pression d'une touche font du NIRS XDS RapidLiquid Analyzer une solution aussi fiable que simple pour le contrôle qualité en laboratoire et en production. Les échantillons sont présentés dans des cuvettes en quartz réutilisables ou des flacons en verre à usage unique ; une chambre à échantillons tempérée assure la reproductibilité des conditions d'analyse et, par conséquent, l'exactitude des résultats de mesure.



### Vision Air 2.0 Complete

**Vision Air - logiciel universel de spectroscopie.**

Vision Air Complete est une solution logicielle moderne et simple d'utilisation pour une application dans un environnement réglementé.

Aperçu des avantages de Vision Air :

- Des applications logicielles individuelles avec interface utilisateur adaptée sont le garant d'un maniement intuitif et simple
- Établissement et suivi simples des procédures de travail
- Base de données SQL pour une gestion sûre et simple des données

La version Vision Air Complete (66072208) comprend toutes les applications d'assurance qualité par spectroscopie Vis-NIR :

- Application de gestion des instruments et des données
- Application de développement de méthodes
- Application d'analyse de routine

Autres solutions Vision Air Complete :

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)