

Bromine number in pyrolysis gasoline

Fast determination of bromine number without chemicals

Pyrolysis gasoline (pygas) and its distillate fractions often contain high levels of reactive unsaturated compounds, making it unusable as a motor fuel. In addition to the amount of diolefins (determined by the Diels-Alder method), the total amount of aliphatic olefinic components also need to be monitored. The standard method to quantify the degree of unsaturation (bromine number) in unsaturated hydrocarbons is titration.

This wet chemical method requires cooling of the sample below 5 ° C to minimize side reactions like oxidation or substitution. In contrast to the primary method, near-infrared spectroscopy (NIRS) needs no sample preparation and is able to determine the bromine number within one minute. NIRS technology fulfills ASTM norms D8321 and D6122.

EXPERIMENTAL EQUIPMENT

180 pygas samples were analyzed on a Metrohm DS2500 Liquid Analyzer equipped with 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 glass vials with a pathlength of 8 mm were used, which made a cleaning procedure unnecessary. Data acquisition and prediction model development were performed with the software package Vision Air complete.



Figure 1. DS2500 Liquid Analyzer.

Table 1. Hardware and software equipment overview.

Equipment	Metrohm number
DS2500 Liquid Analyzer	2.929.0010
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 bromine number determination in pygas. To verify the quality of the prediction model, correlation

diagrams were created which display the correlation between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) are displayed in **Figure 3**.



Figure 2. Selection of different pyrolysis gasoline Vis-NIR spectra obtained using a DS2500 Liquid Analyzer and 8 mm disposable vials.

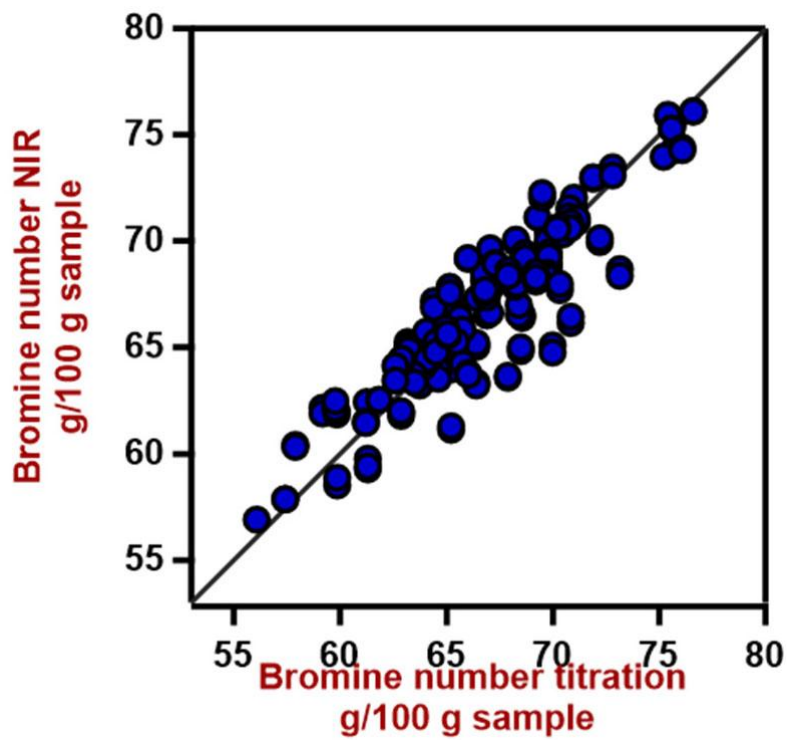


Figure 3. Correlation diagram for the prediction of the bromine number using a DS2500 Liquid Analyzer.

Table 2. Figures of merit for the prediction of the bromine number using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R ²	0.836
Standard Error of Calibration	1.84
Standard Error of Cross-Validation	1.89

CONCLUSION

This application note shows the feasibility of NIR spectroscopy for the analysis of bromine number in pyrolysis gasoline. In contrast to the wet chemical method used in ASTM D1159 (Figure 4 and Table 3), no sample preparation or

chemicals are required with NIR spectroscopy. Aside from the bromine number, additional quality parameters like diene value can be determined in the same sample with NIR spectroscopy.

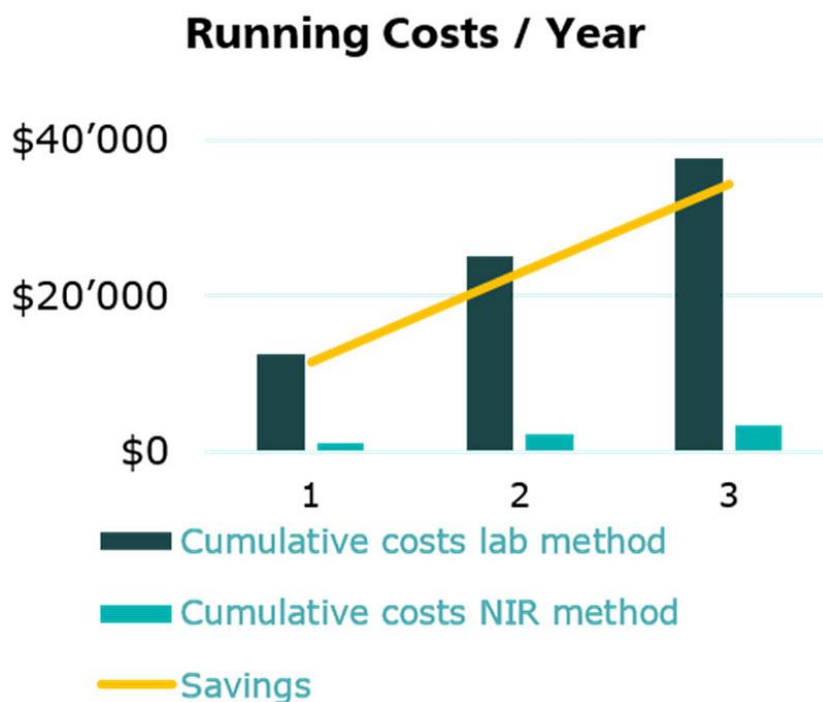


Figure 4. Comparison of running costs per year with the conventional wet chemistry lab method and NIRS.

Table 3. Comparison of costs and time to result (one-fold determination) with the conventional wet chemistry lab method and NIRS.

	Lab method	NIR method
Number of analyses (per day)	10	10
Costs of consumables and chemicals/measurement	\$6	\$0.50
Time spent per measurement	30 min	1 min
Total running costs / year	\$12,533	\$1,125

CONTACT

メトロームジャパン株式会社
143-0006 東京都大田区平
和島6-1-1
null 東京流通センター アネ
ックス9階

metrohm.jp@metrohm.jp



DS2500 Liquid Analyzer

ラボおよび生産環境における品質管理用の堅牢な近赤外分光法。

NIRS DS2500 Liquid Analyzerは、生産チェーン全体に沿った液体のルーチン分析に実績のあるフレキシブルなソリューションです。頑丈な仕様により、NIRS DS2500 Liquid Analyzerは粉塵、湿気、および振動に強い為、過酷な生産環境での使用に理想的です。

DS2500 Liquid Analyzer は400~2500 nmのスペクトル範囲全体をカバーし、サンプルを80° Cまで加熱し、様々な使い捨てハイアルやクォーツキュベットとの互換性を有します。このようにして個々のサンプル要件に対応し得るDS2500 Liquid Analyzerは、1分未満で正確かつ再現性ある結果を得られるようサポートします。さらに一体型のサンプルホルダ検出、および説明不要のVision Airソフトウェアを用いることで、ユーザーが簡単かつ安全に操作できることが保証されます。

サンプル量が多い場合、Metrohmサンプルロケットと組み合わされたフローセルの導入によって、生産性を著しく向上させることができます。



Vision Air 2.0 Complete

Vision Air - 汎用性に優れた分光法ソフトウェア。

Vision Air Complete は、規制環境下での使用のための、操作の容易な最新のソフトウェアソリューションです。

Vision Air の利点の概要:

- 調整済みのユーザーインターフェースを伴う個別のソフトウェアアプリケーションにより、直観的かつ容易な操作が保証されます。
- 作業手順の容易な作成およびメンテナンス
- 安全かつ容易なデータ管理のための SQL データベース

バージョン Vision Air Complete (66072208) には、可視近赤外分光法を用いた品質管理のための全てのアプリケーションが含まれています:

- 装置管理およびデータ管理のためのアプリケーション
- メソッド開発のためのアプリケーション
- ルーチン分析のためのアプリケーション

その他の Vision Air Complete ソリューション:

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



8mmDS2500

直径8 mmのガラス製使い捨てハイアル用インテリジェントホルター