

Application Note AN-PAN-1052

Online process monitoring of octane number during catalytic reforming By NIRS following ASTM D2699 and ASTM D2700

In refineries, high-octane products are desired since they are used to produce premium gasoline. This production is a highly hazardous operation which requires strict adherence to safety standards (IECEx) and constant monitoring of key process parameters such as the octane number (ON). By providing dependable process data in a timely manner, downstream process units (catalytic reformer) can be optimized quickly, increasing profits while lowering operational costs. This Process Application Note presents a way to closely monitor the octane number in fuels in «realtime». Near-infrared spectroscopy (NIRS) technology, which fits well within the international standards (American Society for Testing Materials «ASTM»), makes this possible. This technique offers simple, fast, and reliable online analysis of the octane number, allowing quick adjustments to the process for a better-quality product and higher profitability.



INTRODUCTION

The octane number (ON) is a key parameter measured in the petrochemical refining process which indicates the performance of commercial fuels (e.g., gasoline and jet fuels). It determines the tendency of the fuel to resist auto-igniting in the engine during combustion (knock resistance).

The ON is measured based on the knocking resistance of two reference fuels: iso-octane (C_8H_{18}) and n-heptane (C_7H_{16}). Iso-octane has a high resistance to knocking under harsh conditions and is therefore assigned an ON of 100. Conversely, n-heptane has a low resistance to auto-igniting, thus it is assigned an

ON of 0.

There are two main categories of octane numbers, since the knocking resistance varies based on the operating conditions: research octane number (RON) and motor octane number (MON). The RON is measured under lower temperatures and speeds, and the MON is measured under high temperatures and speeds.

Premium gasoline requires high-octane ingredients. The refining process which produces these highoctane products is called catalytic reforming (**Figure 1**).



Figure 1. Illustration of the catalytic reforming process of naphtha noting suggested online near-infrared spectroscopy (NIRS) measuring point.

Catalytic reforming converts heavy naphtha (a paraffin mixture with low octane rating) into a highoctane liquid product called «reformate» (a mixture of aromatics and iso-paraffins C7 to C10). Therefore, catalytic reforming has a significant impact on the refinery profitability.

The octane numbers of the produced reformate must be constantly monitored to ensure high throughput along the refining process. Traditionally, RON values can be measured by two different methodologies: inferred octane models (IOM) and laboratory octane engine analysis. These methodologies do not provide «real-time» results and require constant maintenance and human intervention to adapt to current operation conditions.

Furthermore, calibration of the octane engine for RON values greater than 100 (a common value for reformate) requires specific blends. These calibrations are not always available. Indeed, refineries often use octane engines to analyze and qualify final blended products (gasoline), with RON between 92–98.



REAL-TIME MONITORING OF OCTANE NUMBERS

«Real-time» analysis of the ON in fuels can be performed online via near-infrared spectroscopy (NIRS), which fits well within the international standards (e.g., ASTM) (Figure 2). However, the reformate stream contains solid particles which interfere with the measurements.

For reproducible and accurate measurements, a preconditioning panel is necessary to filter out the particles and maintain a constant sampling temperature. Additionally, another advantage of using a preconditioning panel is that a sample takeoff point can be implemented as well as a port for validation samples.



Figure 2. Different steps for the successful development of quantitative methods according to international standards.

NIR OCTANE ANALYZER FOR REAL-TIME MONITORING

2060 *The* NIR Analyzers (**Figure 3**) enable comparison of «real-time» spectral data from the refining process to a primary method (i.e., Cooperative Fuel Research «CFR» testing) to create a simple, yet indispensable model for ON monitoring.

Each Metrohm Process Analytics 2060 *The* NIR-Ex Analyzer is configured for applications in ATEX zones. These instruments are capable of monitoring up to five process points per NIR cabinet with the multiplexer option.



Figure 3. The 2060 The NIR-Ex Analyzer from Metrohm Process Analytics.

APPLICATION

After samples are preconditioned, NIR measurements are performed in a flow-through cell. The instruments used in refineries are ATEX or Class 1 Div 1/2 certified. Instruments are either mounted in the refinery where they will require positive air pressure, or in a pressurized shelter. The distance between the instrument/shelter and the sample points can be hundreds of meters.

Every 30 seconds, RON and MON values are transmitted to the programmable logic controller (PLC) or distributed control system (DCS) depending on the communication protocol used.



Table 1. Key parameters and ranges for RON and MON analysis.

	RON	MON
SECV (Accuracy)	0.27	0.15
Precision	0.01	0.01
Range	90–107	80–100
Reference ASTM	D2699	D2700
ASTM Accuracy	± 0.9 (RON 103)	± 1.2 (MON 96)

CONCLUSION

Both monitoring and control of RON and MON in refineries play a crucial role in ensuring the production of high-quality, high-octane products such as premium gasoline.

The use of NIRS technology provides a reliable and efficient method for «real-time» analysis of octane numbers in fuels while aligning with international standards. This enables refineries to optimize their catalytic reforming process quickly, resulting in increased profitability and reduced operational costs. By implementing NIRS technology and utilizing instruments such as the Metrohm Process Analytics 2060 *The* NIR-Ex Analyzer, refineries can achieve better control over their production and improve the quality of their end products.

RELATED DOCUMENTS

Other related documents

<u>AN-NIR-113</u> Research octane number (RON) determination in isomeratev

AN-NIR-114 Determination of RON, aromatics, benzene, olefins, and density in reformate by NIRS

AN-NIR-022 Quality Control of Gasoline

BENEFITS FOR NIRS IN PROCESS

- Optimize product quality (e.g., seasonal effects, crude swing) and increase profit
- Greater and faster return on investment
- Improved product quality and manufacturing efficiency
- Detect process upsets via automated analysis





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CONFIGURATION



2060 The NIR-Ex Analyzer

The **2060** *The* **NIR-Ex Analyzer** is the next generation of process spectroscopy instruments from Metrohm Process Analytics. With its unique and proven design from the inside out, it delivers accurate results every *10 seconds*. It can provide non-destructive analysis of liquids and solids directly in the process line or in a reaction vessel by using fiber optics and contact probes. It has been designed to connect up to five (5) probes and/or flow-cells. All five channels can be configured independently from each other using our versatile embedded proprietary software.

Additionally, this analyzer is IECEx certified and fulfills the ATEX EU Directives. It has been designed with an approved purge/pressurization system together with intrinsically electronic devices, preventing any potentially explosive fumes or gases from the ambient air entering the analyzer enclosure. Furthermore, it is available in three other versions: the 2060 *The* NIR Analyzer, 2060 *The* NIR-R Analyzer, and 2060 *The* NIR-REX Analyzer.

