Boost efficiency in the QC laboratory: How NIRS helps reduce costs up to 90%

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Underestimation of quality control (QC) processes is one of the major factors leading to internal and external product failure, which have been reported to cause a loss of turnover between 10–30%. As a result, many different norms are put in place to support manufacturers with their QC process. However, time to result and the associated costs for chemicals can be quite excessive, leading many companies to implement near-infrared spectroscopy (NIRS) in their QC process. This paper illustrates the potential of NIRS and displays cost saving potentials up to 90%.

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Quality Control with NIR Spectroscopy – A sustainable boost in efficiency

«Good quality is expensive.» One could argue that high product prices are often due to costly production processes, which result from extensive quality control (QC) and quality assurance (QA) measures. However, as a QA/QC Manager, you might disagree and refer to personal examples and scientific studies outlining the consequences of poor quality control measures. The following white paper provides a short summary about the importance of QC and QA, while illustrating action points to improve existing QC processes. Furthermore, near-infrared (NIR) spectroscopy is presented as a powerful analysis technique to increase QC efficiency while maintaining the accuracy and precision of the existing analysis method.

The importance of QC and QA

Two main failure costs are addressed and mitigated with a reasonable QC/QA framework in place:

- Avoidance of internal failure
- Avoidance of external failure

Internal failure costs are associated with internal errors (e.g. re-inspection, rework, or scrapping). External failures are related to product defects found after delivery to the customer. These are expensive and involve a significant risk because they can affect brand reputation or even induce a loss of market share. Follow-up actions such as warranties, repairs, or recalls, require a great expenditure and therefore will significantly reduce revenues.

To avoid these failures and their related costs, it is advisable to invest reasonably into prevention measures. One such activity is the continuous monitoring of used raw materials, intermediate products, and final products. More commonly, companies prefer to gamble by under-investing in this area and neglect the negative implications, which can result in a loss of turnover between 10–30%.[1]

Aside from implementing the appropriate checks along the complete production process, companies should also challenge their existing QC processes and setups in order to discover how to further increase production efficiency. Possible approaches include:

- Reduce budget for testing and inspection
- Increase efficiency of production equipment
- Improve productivity of the operators
- Make manufacturing easier

One strategy could be to analyze each of these action points individually, in order to find any major gaps as well as to define the respective countermeasures. Alternatively, companies can also take advantage of more modern QC technologies which have the potential to address all four of these approaches directly.

Near-Infrared Spectroscopy (NIRS) is an example of a modern QC method which significantly boosts the efficiency of QC labs. In the following section, this technology and its benefits are presented and discussed.

Near-Infrared Spectroscopy (NIRS)

All spectroscopic methods determine sample properties by analyzing the specific interaction between light and matter. This interaction varies in dependence of the applied light source, and therefore the different spectroscopic technologies are defined by the applied light energy (i.e. wavelength), and by the type of interaction. With NIRS, for example, instruments detect the quantity of absorbed (absorbance spectroscopy) near-infrared light (NIR = 800–2500 nm respectively 12500–4000 cm^{-1}, see **Figure 1**) by functional groups such as -CH, -NH, -SH, or -OH.

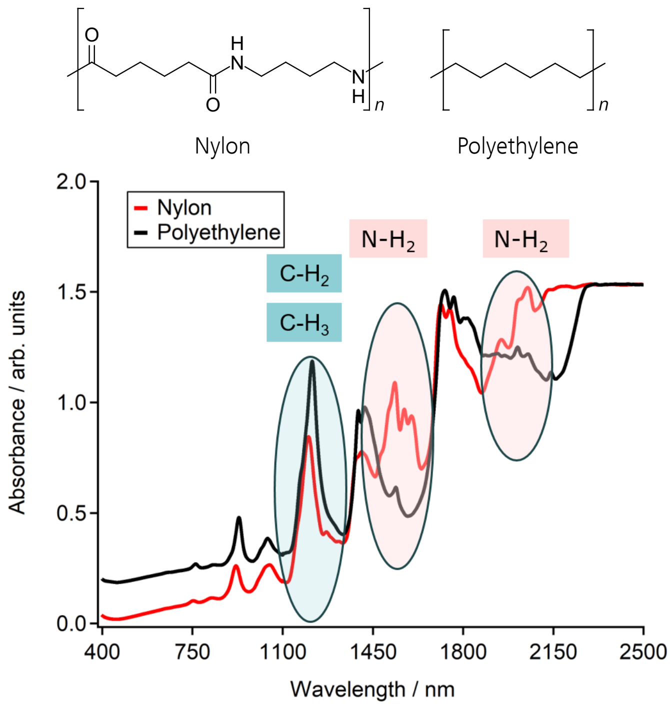

Figure 1. Comparison of spectra taken from Nylon and polyethylene in the near-infrared wavelength region. The differences seen are due to their different chemical structures – Nylon contains nitrogen functional groups whereas polyethylene does not.

Since the NIR light-matter interaction is by nature fast and non-destructive, NIRS-based analytical methods offer significant advantages over conventional approaches. Samples are analyzed as-is without time-consuming preparative steps, and remain undamaged. All NIR-sensitive information is gathered by a single measurement in less than one minute, and is displayed in the spectroscopy software as a spectrum.

The action of acquiring a quick and complete overview of information is identical to the experience of capturing the image of an object with a camera. A single picture includes all sorts of information about the object e.g. color, size, shape, position, etc. Analogous to the picture, a spectrum is a complete scan which includes numerous information about the sample (e.g. the water content, OH-Number, viscosity, or the acid number). For both the camera image and sample spectra, the only necessary action is to interpret the data, which in the case of NIRS is performed by the provided manufacturer spectroscopy software.

Currently, manufacturers of NIR instruments pay particular attention to the convenience of system operation, resulting in standardized analyzers and easily defined operating procedures. Both facets simplify the implementation of NIR spectroscopy into daily QC operations, **even across multiple locations**, requiring only minimal training of the operators.

In regards to the action points to improve QC efficiency on the previous page, it is apparent that companies which have implemented NIRS methods into their routine QC testing are able to reduce their testing budget and improve their operators' efficiency at the same time. **Table 1** and **Figure 2** present the potential return on investment (ROI) by comparing analysis costs per year between the commonly used methods of titration and viscometry versus near-infrared spectroscopy.

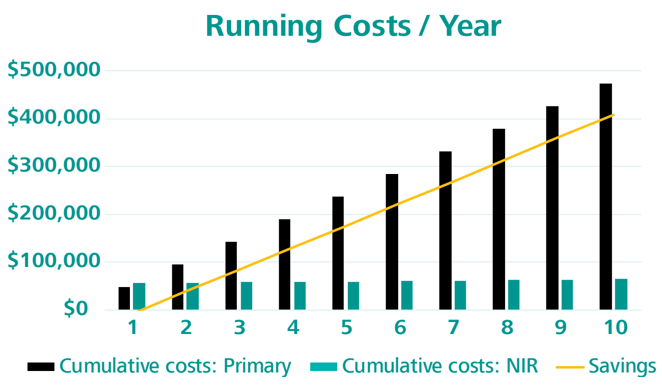

Figure 2. Possible return on investment as related to running costs when analyses are conducted with NIRS vs primary methods.

Table 1. Overview of estimated costs for the analysis of different parameters with primary methods vs NIRS. The full ROI is achieved within 11 months.

Total analyses per day	10	10
Cost of operator per hour	$ 25	$ 25
Cost of Analyzer	**Primary Method**	**Near-Infrared Spectroscopy**
DS2500 Analyzer	—	$ 55,000
Total initial costs	$ 0 [1]	$ 55,000
Running costs consumables and/or chemicals: per analysis		
Determination of H_2O content (**ISO 15512**)	$ 5	$ 0
Determination of functional groups	$ 5	$ 0
Determination of viscosity (**ISO 307**)	$ 6	$ 0
Total costs consumables and/or chemicals: per year	$ 35,100	$ 0.00
Time spent per analysis (minutes)		
Determination of H_2O content (**ISO 15512**)	5.0	0.5
Determination of functional groups	5.0	0.5
Determination of viscosity (**ISO 307**)	15.0	0.5
Total yearly labor costs	$ 23,438	$ 469
Total running costs	**$ 58,538**	**$ 469**

[1]Assumption that the instrument had previously been purchased, and therefore this cost is not included in the ROI calculation.

Application Examples

Some key parameters have already been mentioned in the previous chapter, however a complete list of possible NIRS applications would exceed the scope of this paper. Typical industries where NIRS is an established analytical QC method include:

- chemicals
- lubricants
- petrochemicals
- polymers
- paint, inks, and dyes
- pulp and paper
- pharmaceuticals
- personal care and cosmetics
- food and feed, agriculture

In the following section, three different industries and application examples are described. However, it is important to note that the precision values are a function of the chosen concentration range. Therefore, selecting lower concentration ranges will most likely further enhance the precision of the results.

Chemical Industry – Polyols

Polyols, a class of organic compounds characterized by the presence of two or more hydroxyl groups, are crucial starting materials for the production of polyurethanes. Both the reaction behavior of polyols and the composition of the final product are highly dependent on the number of hydroxyl groups, which makes the analysis of this functional group so important. The reactivity of polyols also depends upon their moisture content and the acidity represented by the number of attached carboxylic acid groups.

NIRS is an established technology for the analysis of polyols (**ASTM D6342**), able to precisely determine all three parameters within 30 seconds as shown in several applications [2]. Table 2 presents some key results from a polyol analysis utilizing NIR spectroscopy.

Table 2. Overview of typical parameters measured in the polyol industry which can also be analyzed by NIR spectroscopy.

Parameter (unit)	Range	Precision
Hydroxyl Value (mg KOH/g)	70.00–125.00	0.68
Acid Value (mg KOH/g)	0.10–8.00	0.38
Moisture content (mg/L)	75–400	52

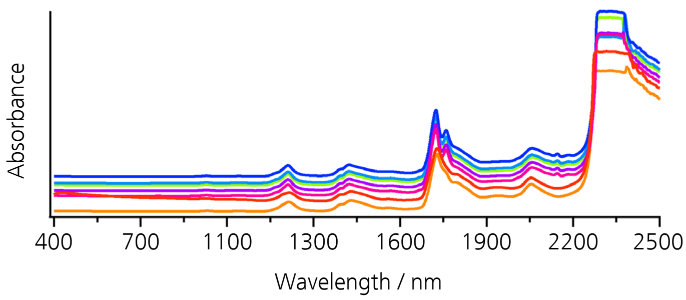

Figure 3. NIR spectra taken of polyol samples with varying OH number values.

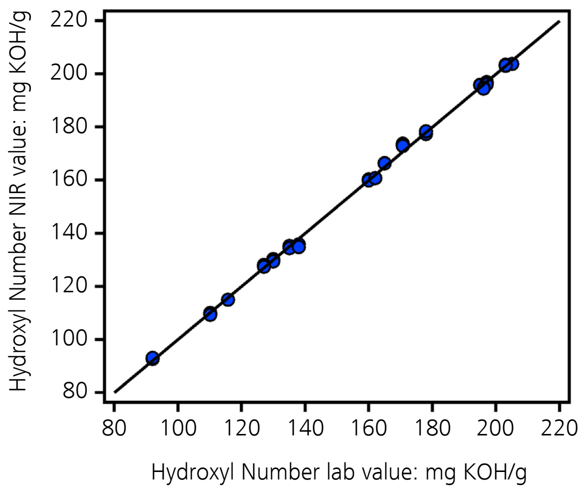

Figure 4. Correlation plot comparing NIRS to a primary laboratory method.

Polymer Industry – Polyethylene terephthalate

Polyethylene terephthalate (PET) is one of the most produced polymers worldwide, next to polyethylene and polypropylene. Raw materials for the production of PET include diethylene glycol along with either dimethyl terephthalate or terephthalic acid during transesterification and esterification reactions.

Product quality is primarily determined by the content of diethylene glycol (DEG) and isophthalic acid (which reduces the crystallinity of PET). Additionally, the intrinsic viscosity (IV) (**ASTM D4603**) and the acid number (AN) are important parameters to control in order to avoid external failures. NIRS has proven its validity as an analytical method which reliably determines these parameters. **Table 3** displays the respective concentration ranges and precision values for this application as described in the Metrohm Application Note NIR-023 **[3]**.

Table 3. Overview of typical parameters measured in the polymer industry which can also be analyzed by NIR spectroscopy.

Parameter (unit)	Range	Precision
Diethylene glycol content (%)	1.4–2.0	0.066
Isophthalic acid content (%)	1.8–4.5	0.143
Intrinsic viscosity	0.5–0.9	0.024
Acid number	1.2–6.0	0.143

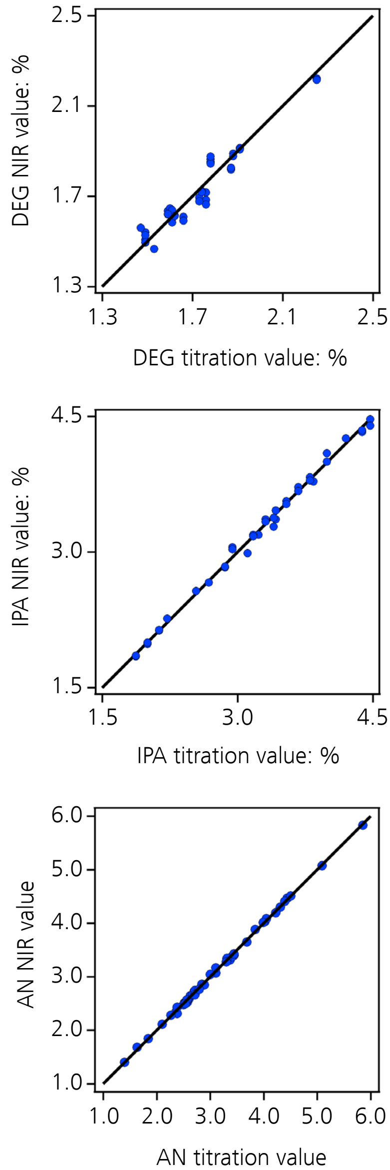

Figure 5. Correlation plots for NIRS compared to laboratory primary methods for diethylene glycol (DEG), isophthalic acid (IPA), and acid number (AN).

Petrochemical Market – Gasoline

Gasoline is one of several end products resulting from a complex production chain starting with the refinement of crude oil. This fuel product requires intensive checks on several quality parameters which need to be within specification before commercialization. These parameters, which can also be controlled by NIR analysis include the Research Octane Number (RON) and Motor Octane Number (MON), the olefins, oxygen, aromatic content, and the density.

The importance of measuring these values precisely is not just related to regulations, but this also offers manufacturers further potential to save costs. As an example, RON values exceeding the requirement will still be accepted by the market, but these products include a higher amount of lucrative long-chain organic molecules. This so-called «RON give away» (**Figure 6**) is estimated at approximately **0.5 RON per barrel**, resulting in **2.25 million USD/month** in lost revenue for a production of 100,000 barrels per day.

Ready-to-use NIRS systems are available for monitoring several gasoline parameters, which cover varied ranges and their respective precisions, shown in **Table 4**. Additionally, the manufacturers of NIRS analyzers usually offer application support to extend these ranges or improve upon the precision.

Table 4. Overview of typical parameters measured in the petrochemical industry which can also be analyzed by NIR spectroscopy.

Parameter (unit)	Range	Precision
RON	85.00–94.00	0.68
MON	81.00–100.00	0.53
Olefins (%)	1.0–25.0	1.3
Oxygen (%)	0.200–2.000	0.045
Aromatics (%)	20.0–45.0	1.1
Density (g/cm^3)	0.7400–0.7600	0.0024

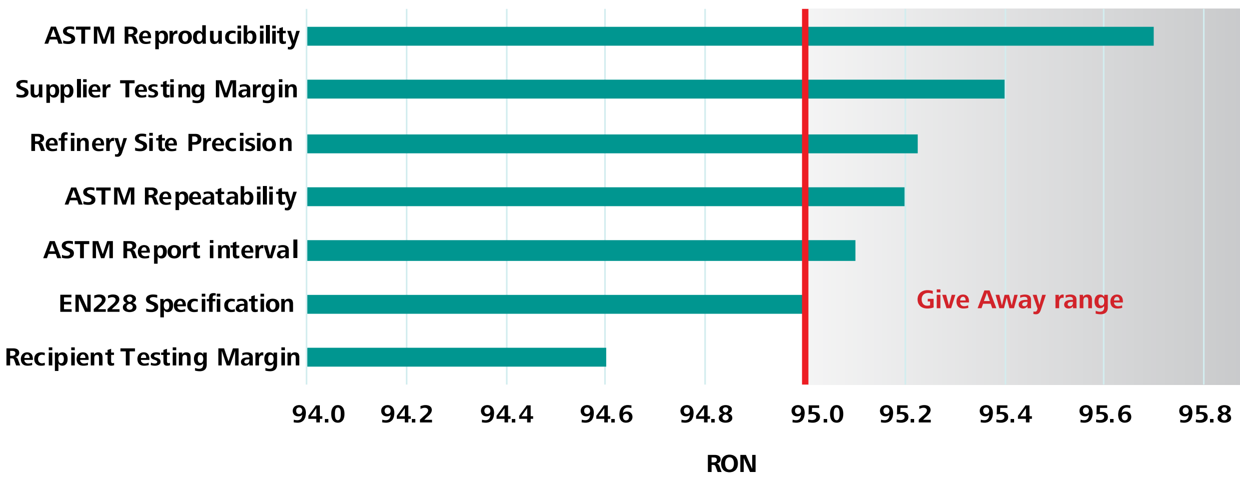

Figure 6. Overview of typical RON give aways in relation to different methods.

Summary

At first glance, investment into quality control might increase product costs. However, this reduces costs related to external and internal failures, which are of higher magnitude and have the potential to reduce up to 30% of the turnover.

Besides enforcing a reasonable quality control program, the efficiency of the QC and QA department is required to produce materials cost-effectively. One way to achieve this is to implement modern, easy to use, fast QC methods. NIRS is an established methodology used across different industries. This technique combines these requirements and provides significant potential to reduce costs and increase operator efficiency.

References

[1] Why Improving Quality Leads to Lower Manufacturing Costs, QualityInspection.org. (accessed October 30, 2019). https://qualityinspection.org/improving-quality-cost-china/

[2] Metrohm Application Note **NIR-035** Hydoxyl number in liquid polyols using Vis-NIR spectroscopy https://www.metrohm.com/en/applications/AN-NIR-035

[3] Metrohm Application Note **NIR-023** Diethylene glycol, isophthalic acid, intrinsic viscosity, and acid number in PET granulate by NIRS https://www.metrohm.com/en/applications/AN-NIR-023

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