NEO Monitors

IROSS™

IN-SITU
REAL-TIME
OVERLAPPING
SPECTRAL
SEPARATION

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/ MULTI-COMPONENT MEASUREMENTS USING IROSS™

Since the first TDLAS analyzers successfully made the step from the laboratory to industry in the 1990s, this innovative technology has undergone tremendous development. Following Roger's "Diffusion of Innovation" theory (1), it was first the *innovators* and then the *early adopters* who ventured to install a TDLAS analyzer. Today, the technology is in the midst of being used by the *early majority* in a growing number of applications in many industries. This means that TDLAS is currently experiencing great momentum. Nevertheless, further improvements and new innovations are needed to maintain this momentum and also reach the *late majority* in the future.

Initially, the technology was restricted to a few gases and applications due to the limited wavelength coverage and usability of the semiconductor laser source. Today, it is possible to get a good and reliable laser for essentially any wavelength in the infrared spectral range. This enabled more than a hundred different applications, and TDLAS has become the standard technology for many of them.

A traditional TDLAS analyzer uses a single laser source and can typically measure one or two, perhaps three gas components, depending on the availability of interference-free absorption features of the targeted gases within the limited tuning range of the laser. Recently, however, there has been an increasing interest from many industrial customers to measure more components in order to obtain all the necessary information for proper process control, the combination of process control and safety as well as for emission monitoring applications.

This poses a new challenge for TDLAS technology and has triggered several new developments and innovations. Looking at the options for measuring multiple components, the following three are available:

- The most obvious option is to simply increase the number of analyzers installed at the measuring point. Although this is feasible, as the installation shown in Figure 1 in an Arkema Forane plant near Lyon (France) demonstrates, it is not a very elegant and efficient solution.
- Alternatively, several laser sources can be integrated into a single analyzer. This was first applied in combustion analysis to combine oxygen (O_2) and carbon monoxide (CO) measurements in a single transceiver device (2). Here, two lasers are required as the absorption features of the two species are too far apart to be measured with a single laser source. This has proven to be a powerful option and is now standard for many heater and burner applications.
- And then there is the option of using modern signal processing to extract more information than before from the process gas spectrum recorded with a single laser. More computing power and major advances in modern signal processing have made this option possible. The advantage of this approach is that more information can be extracted for the same cost of goods and services, as no additional hardware or installation is required.

Figure 1: Five TDLAS analyzers mounted on a stack.

As with many developments, it can be very helpful to take inspiration from other areas. The TDLAS variant wavelength modulation spectroscopy (WMS), for example, uses techniques that were originally conceived for radio communication.

This paper will illustrate how the music industry has inspired the development of a new signal processing algorithm that has significantly extended the capabilities of TDLAS without sacrificing its advantages. Finally, three examples will be presented in which the algorithm is already being used in important applications.

/ In-Situ Real-Time Overlapping Spectra Separation

The selection of laser wavelength is an essential part of any TDLAS application assessment and is critical to a properly functioning analyzer. Customers want to be sure that they can rely on the measurement results, achieve the required sensitivity and that there are no interfering signals from other gases in the process.

Normally, the laser wavelength is chosen so that an isolated absorption feature can be measured (traditional single-line TDLAS). In some cases, e.g., the measurement of O_2 at around 760 nm, this is easily accomplished. But for other gases finding isolated absorption features can be a very difficult task. Strongly absorbing and omnipresent species, such as water vapor (H_2O), methane (CH_4) and carbon dioxide (CO_2) can completely obscure the gas of interest, especially at high temperatures. This is known as spectral interference and is often the limiting factor when it comes to feasibility, selectivity and sensitivity of a TDLAS measurement.

If several species absorb in the same scanning range of a laser, the recorded spectrum can be considered as a linear combination of the individual spectra; the latter is referred to below as a "composite spectrum". The industry standard to address interferences is curve-fitting. This is based on a detailed molecular absorption database like HITRAN (3) together with a physical model that accurately describes the absorption of light through interaction with a gas mixture. By knowing the properties of the gas (temperature, pressure, gas composition, etc.), the best fit of the model to a measured spectrum can be calculated through an iterative, error-minimizing procedure.

An alternative approach is to split the composite spectrum into separate spectra for the target species so that each can be processed individually to calculate a gas concentration as well as extract other process information. A key factor in the development of a new algorithm is that the advantages of TDLAS technology, in particular sensitivity and real-time responses, are preserved.

Such a task is not specific to TDLAS, and similar challenges can be found in other sectors including the music industry. Nowadays, it is very common for band members not to be in the same studio at the same time when recording a new song. Instead, separate tracks are recorded for each instrument and vocal. A mixer merges all the tracks together with volume adjustments to create the final song (Figure 2). In this analogy, the song is the composite spectrum.

Fortunately, the music industry has also developed tools for the reverse process that can be used to separate the individual instruments and vocals of a song. This is called "source separation" and the same principle can be applied to a composite spectrum.

NEO Monitors' IROSS™ (in-situ real-time overlapping spectral separation) signal processing technique is a modified source separation algorithm tailored to the needs of separating a composite spectrum into individual spectra in real-time. These spectra are then processed separately by traditional TDLAS signal processing procedures.
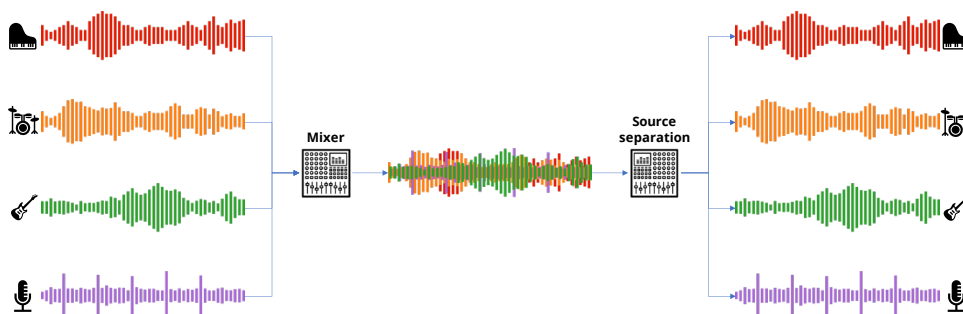

Figure 2: Schematic depiction of combining four audio tracks into one song via a mixer and then using source separation to extract the individual tracks from the song again.

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For the new algorithm, the aforementioned molecular database model was replaced by a library of actual measured spectra. This was done since databases are not always complete (e.g., missing absorption lines or even whole wavelength regions, missing information about line broadening, etc.) or sufficiently accurate for the purpose. Complex digital filtering of the measured spectra can be difficult and time-consuming, and a non-linear scanning frequency of the laser source is difficult to model which means that a detailed measurement of the laser scanning frequency would be required.

The raw library contains many spectra for different process conditions (temperature, pressure, gas composition, etc.), so that the task of separating spectra in real-time would be a challenge even for powerful desktop computers. The library is therefore compressed using principles of multivariate analysis. Since the measured spectra differ only slightly in width, amplitude and position, it is obvious why this is possible.
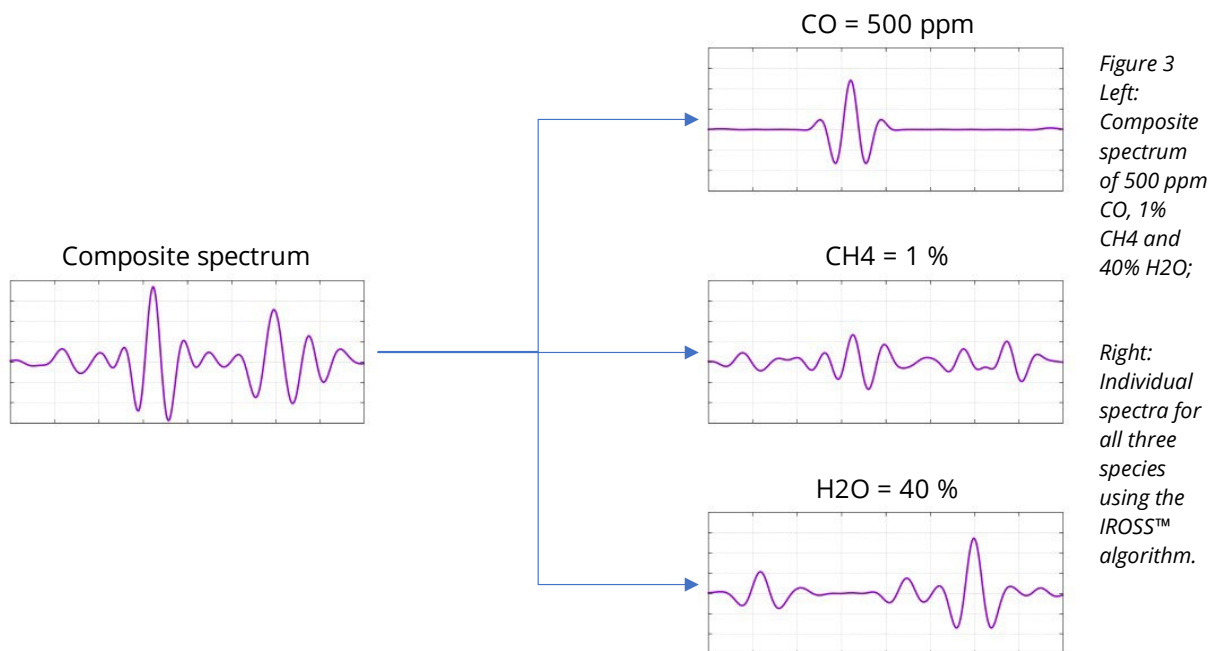
Crucial for the reliability of the algorithm is that, by design, it cannot produce fits beyond the recorded library and is therefore capable of detecting any variations in the measured spectrum that is outside the boundaries set by the pre-collected library.

Three examples of successful applications of the algorithm are presented below. These examples demonstrate the algorithm's flexibility and ability to be applied to various gas combinations and process conditions across different industries.

/ Example: Combustion

The first application that historically led to the development of the new algorithm is the control of combustion processes. As laboratory and field measurements at high temperatures (above 600 °C) show, the commonly used CO absorption line suffers from interference from CH_4. Thanks to the new algorithm, this challenge was solved, opening new possibilities for end users, as the application example below will show.

Figure 3 illustrates the application of the source separation algorithm. The left-hand side shows the composite spectrum of CO, CH_4 and H_2O, while the right-hand side shows the separated spectra with the respective concentration values.

CO = 500 ppm

Composite spectrum

CH4 = 1 %

H2O = 40 %

Figure 3 Left: Composite spectrum of 500 ppm CO, 1% CH4 and 40% H2O;

Right: Individual spectra for all three species using the IROSS™ algorithm.

The practical suitability of the algorithm was recently demonstrated in a natural gas-fired process heating system (4). A combined CO and CH_4 analyzer was installed alongside an O_2 analyzer. Since O_2 absorbs in a completely different wavelength region than CO and CH_4, a separate analyzer must be used for this measurement. The process temperature was 700 °C and the optical path length was 27 m.

The CH_4 measurement was primarily intended to detect CH_4 when the heater was switched on and off. However, the operators soon discovered that the analyzer was detecting rising CH_4 levels during normal operation. It can be seen from Figure 4 that there is an immediate CO breakthrough when O_2 levels are reduced, as would be expected, followed by an increase in both CO and CH_4 levels when higher fuel levels are introduced, while maintaining very low O_2 levels.
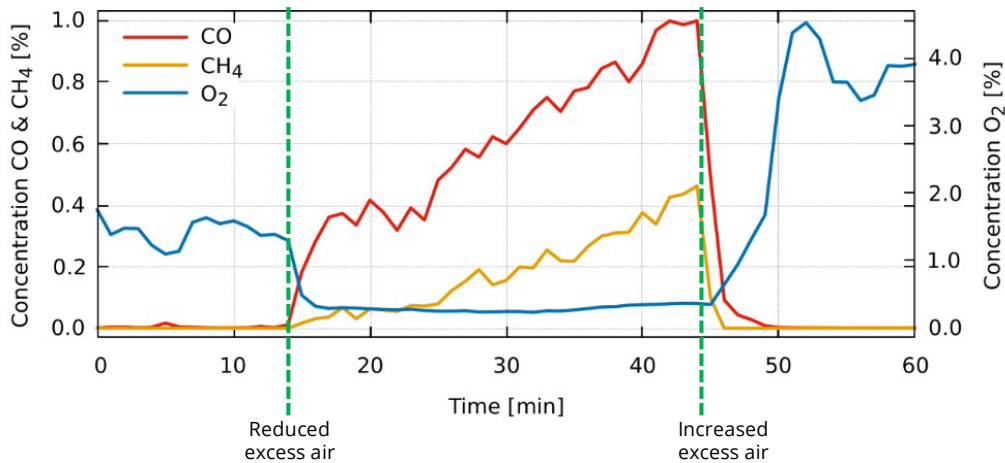

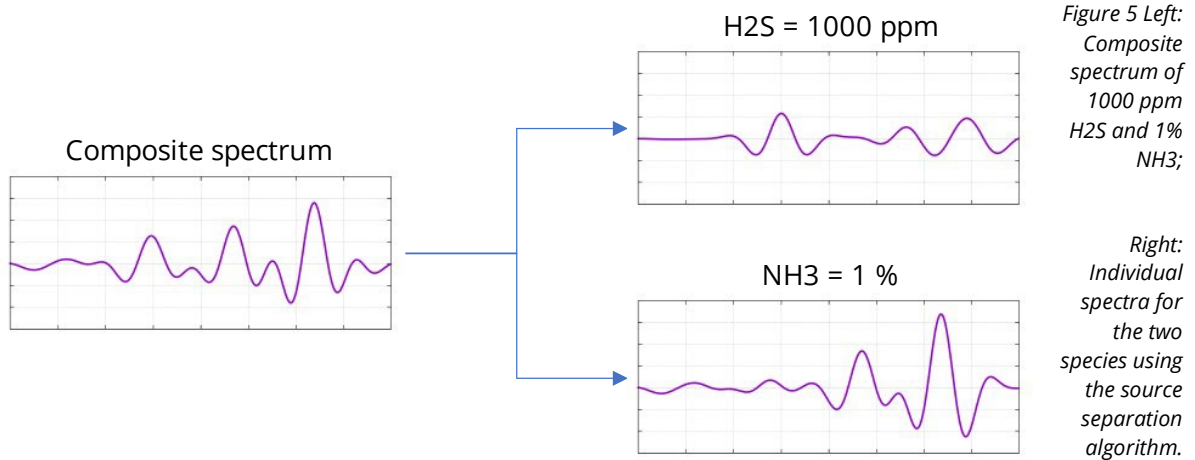*Figure 4: Concentration plot of CO and CH4 (left y-axis) and O2 (right y-axis).*

Combustion was still occurring under these conditions, but not to completion. However, there was no flame-out situation. From this specific operating profile, under such conditions, CH_4 can indeed be present in the heater, even during what is considered a normal operating cycle. The autoignition temperature of CH_4 is approximately 600 °C. Therefore, it is typically assumed that unburnt fuel would not be present under normal operating temperatures, as it would be completely combusted. However, this autoignition temperature is defined for stoichiometric mixture with oxygen. The reduced O_2 levels present within the process heater cause the autoignition temperature to increase.

This phenomenon was unknown to the operator, but thanks to the algorithm, they can now combine process control (CO measurement) and safety (CH_4 measurement) in a single TDLAS analyzer.

/ Example: Coke oven gas

Coal is a primary raw material in the steel industry. In a process known as coking, a mixture of different types of coal is converted into coke. Coke oven gas (COG) is a valuable by-product that serves as an energy substitute for natural gas. However, the raw COG contains impurities such as hydrogen sulfide (H_2S) and ammonia (NH_3). These substances can lead to corrosion of pipelines and equipment, poison the adsorbents and catalysts of scrubbers and produce sulfur oxides (SOx) and nitrogen oxides (NOx) when COG is burned. H_2S and NH_3 are therefore removed from the COG and the residual gas concentrations are measured downstream of the scrubbers. Unfortunately, H_2S generally suffers from strong NH_3 interferences, which can lead to larger offsets and might render the measurements unusable. Again, applying the source

separation algorithm helps not only to remove the NH_3 interference from H_2S, but also to make both gas concentrations available in a single unit for the end user. Figure 5 shows laboratory measurements for illustration purpose.

H2S = 1000 ppm

NH3 = 1 %

Composite spectrum

Figure 5 Left: Composite spectrum of 1000 ppm H2S and 1% NH3;

Right: Individual spectra for the two species using the source separation algorithm.

/ Example: DENOX

Selective catalytic reduction and selective non-catalytic reduction are commonly used methods to remove NOx from the off-gas of industrial processes. NH_3 is used as a reducing agent, optionally with the involvement of a catalyst, to convert NOx into nitrogen (N_2) and H_2O.

Following the chemical reaction, H_2O concentrations can be very high, even up to 60% or more in certain installations. When this occurs, the NH_3 line broadening due to H_2O is significant and the resulting concentration measurement will deteriorate if the effect is not properly compensated. While it is possible to measure the line-width at higher NH_3 concentrations and compensate for the broadening effect, this is not possible at low concentrations. In this case, the nearby H_2O water line can be used to measure the concentration to compensate for the broadening of the NH_3 line. A laboratory measurement of 2 ppm NH_3 and 60% H_2O (Figure 6) also shows that H_2O creates an offset in the NH_3 measurement that is very difficult to remove with traditional TDLAS signal processing.
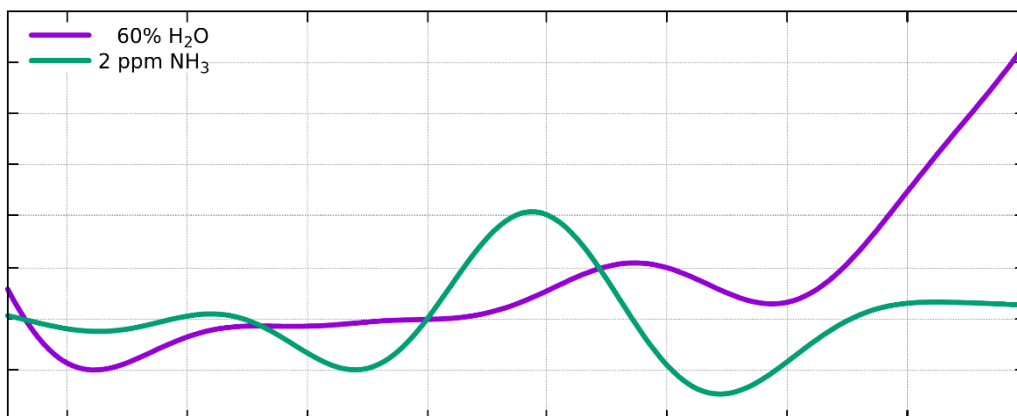

Legend:
- 60% H_2O
- 2 ppm NH_3

Figure 6: Recorded spectra of 2 ppm NH3 and 60% H2O.

However, the source separation algorithm can separate the two spectra so that NH_3 can be measured without interference and the additional measurement of the H_2O concentration can be used to compensate for line broadening effects (Figure 7).

NH3 = 5 ppm
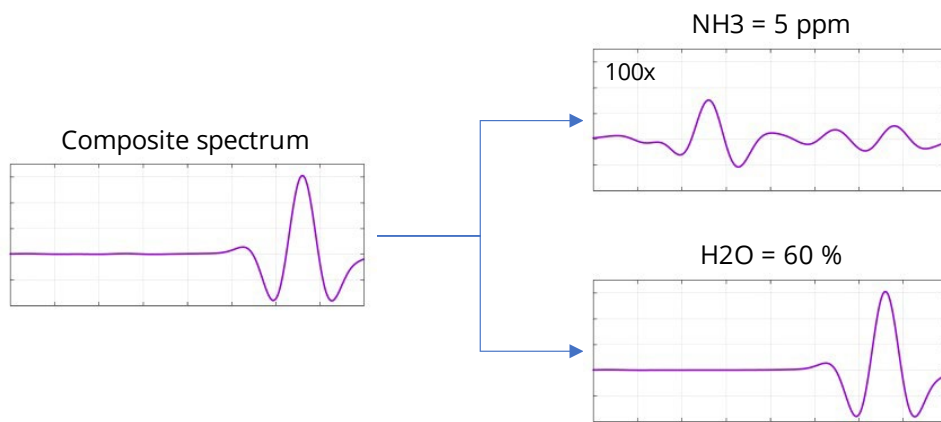
100x

Composite spectrum

H2O = 60 %

Figure 7 Left: Composite spectrum of 5 ppm NH3 and 60% H2O;

Right: Individual spectra for the two species using the source separation algorithm. The NH3 spectrum was scaled by a factor of 100 for better visibility.

Figure 8 shows laboratory NH_3 measurements with different H_2O backgrounds. For this purpose, a sample cell was filled with 4 ppm NH_3 in nitrogen (N_2) as balance gas. Different H_2O concentrations (purple trace, right y-axis), varying between 3% and 21%, were added to the balance and the measured NH_3 spectra recorded. The spectra were processed in three different ways, corresponding to three different configurations of the analyzer, as described in the following: The orange trace (left y-axis) shows the measured NH_3 concentration with traditional signal processing and without compensation for the line-broadening induced by the added H_2O; at this low signal levels, a reliable line-width measurement is not possible. As expected, the NH_3 concentration is underestimated when only the line-amplitude is used in the signal processing.

The blue trace shows the measured concentration when the analyzer is set to a fixed H_2O value; in this case 15%. Here, the analyzer constantly compensates for a pre-configured line-broadening. As can be seen, the NH_3 is measured correctly when 15% H_2O are added, but NH_3 is over- or underestimated, respectively, for other H_2O concentrations.

Finally, when IROSS™ is activated, the NH_3 concentration is measured correctly regardless of the actual H_2O concentration. Thanks to the additional H_2O measurement, the line-broadening can be dynamically compensated.
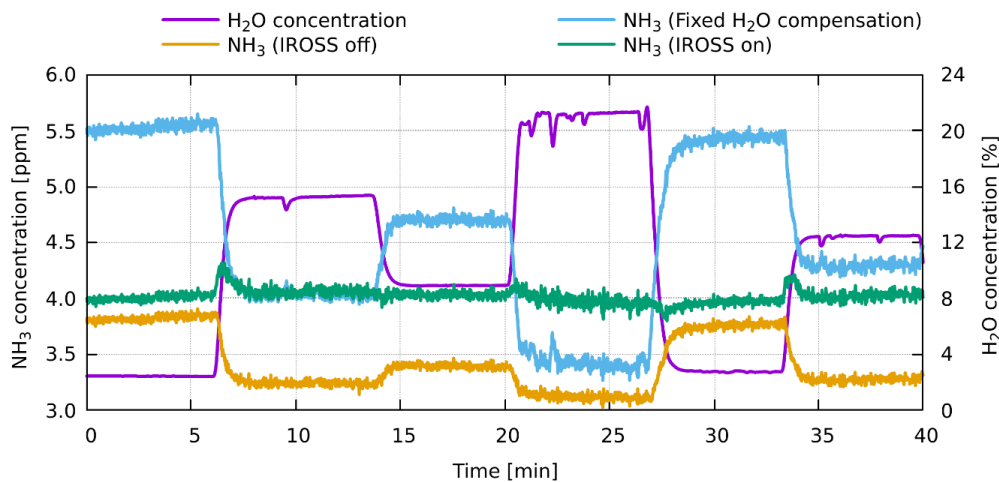

Figure 8 Concentration measurements of NH3 in N2 with different H2O backgrounds and with different measurement configurations.

/ Conclusions

In summary, modern signal processing can significantly expand the capabilities and application range of TDLAS analyzers. Inspired by the music industry, a source separation algorithm can be adapted and optimized so that composite spectra can be separated into individual spectra. In this way, interference can be reduced, and more information than before can be extracted from a single laser spectrum. As the three application examples show, such an algorithm can be used very flexibly for completely different applications in various industries. The new possibilities gained in this way allow real-time multi-component measurements with more specific and precise results and, thanks to additional information, also allow combined purposes such as process control and safety.

/ References

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3. Gordon, I.E., Rothman, L.S., Hargreaves, R.J. et al. "The HITRAN2020 molecular spectroscopic database", Journal of Quantitative Spectroscopy and Radiative Transfer 277, 107949 (2022)
4. Rye, S. "Safe combustion", Hydrocarbon Engineering, August 2023

/ About us

NEO Monitors AS was founded in 2003 as a commercial part of Norsk Elektro Optikk AS (NEO).

Today, NEO Monitors is a leading manufacturer and supplier of TDLAS gas and dust analyzers, based on over 30 years of high-risk research and development in electro-optics and laser technology.

NEO Monitors develops and supplies tailored solutions (LaserGas™ and LaserDust™) for measuring gas and dust in all types of industries worldwide.

The solutions have three main missions:

1. Optimize production processes.
2. Control and improve safety.
3. Measure emissions.

The analyzers can measure over 40 gases and combinations and are used in numerous kinds of applications in all kinds of industries, such as cement, chemical/petro-chemical, oil and gas, power, pulp and paper, environmental, fertilizer and many more.

NEO Monitors has more than 40 distributors spread across all continents. It is the fastest growing European company in this niche, with over 20.000 analyzers installed (2024).

The analyzers accommodate different needs in the industry, from monitoring gas in stacks, pipes, ducts and process chambers to monitoring the safety of workers and environmental functions.

NEO Monitors AS was acquired by the Nederman Group in 2017 and we are proud to represent the same values:

"We protect people, planet and production from harmful effects of industrial processes, contributing to sustainable production, environmental benefits and a safe workplace."

/ Our Distributors

NEO Monitors' solutions and expertise are available from a global distributor network.
Our partners ensure that resellers and customers all around the world have access to our solutions, help them with the implementation and offer service, training and support.

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