

# REACH Compliance with Near-infrared and Raman Spectroscopy Tools

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## Introduction

On June 1, 2007, a new European Union regulation regarding chemical safety came into force. This regulation named “Registration, Evaluation, Authorization and Restriction of Chemicals” (REACH) is designed to ensure all chemicals used in the European Union have been properly tested and safely used. This far reaching complex regulation affects all chemical producers worldwide even if they do not have business with members of the European Union. Thermo Fisher Scientific is committed to assisting chemical producers and manufacturers comply with REACH through the use of the Thermo Scientific Antaris near-infrared (NIR) and Thermo Scientific DXR SmartRaman analytical instruments.



Figure 1: The European Union’s REACH legislation to establish human exposure and environmental release guidelines for all chemicals used in Europe has worldwide implications.

The REACH legislation grew from the need to replace the patchwork of existing laws in several European countries with one comprehensive, all-encompassing regulation. A further complication of the existing regulations was the segregation of chemicals into those introduced before or after 1981. Chemicals introduced after 1981 have been subject to more careful testing and labeling than older

chemicals which were exempted from the rigorous scrutiny. The testing standards from 1981 proved to be largely ineffective because over 100,000 chemicals were exempt which accounted for virtually all of the industrial materials in use. The REACH initiative will require registration and testing of these pre-1981 chemicals as well as any newer ones.

REACH was first proposed in 2001 to allow for preregistration of chemicals from June 1, 2008 until December 1, 2008. Beginning on January 1, 2009 and continuing over the next 11 years, the full registration and testing process will occur. New chemicals will be continually added and tested indefinitely. Registration, testing and labeling will first concentrate on large volume chemicals and those suspected of being most hazardous (Substances of Very High Concern); subsequent stages in the process will focus on those chemicals used in lower volumes.

The process required companies to preregister any chemical they might want to market after January 1, 2009. However, due to the high traffic on the established website, the European Chemical Agency suggested companies only preregister those chemicals they definitely intended to market. Nevertheless, several companies preregistered the entire European Inventory of Existing Commercial Substances; more than 100,000 chemicals. This was a move to ensure products that contain multiple substances, including unknown ones, could still be marketed. The sheer amount of analytical work that will be involved in testing this large number of chemicals will require tools to rapidly identify and characterize single substances as well as multiple components in mixtures. The Thermo Scientific NIR and Raman instruments are specifically designed to collect important chemical information rapidly and consistently which makes them useful in several places during the process.

A key component of simplifying this process is the assignment of chemicals into Substance Information Exchange Forums (SIEFs). Manufacturers, importers, and customers will be assigned to SIEFS and are expected to cooperate on gathering and processing data on the specific chemicals. This cooperation may be difficult to achieve as the cost of testing and the value of data is difficult to equitably assign. A likely resolution will be to share the costs of independent analysis and analytical equipment.

## Key Words

- Antaris
- DXR SmartRaman Spectrometer
- FT-NIR
- Raman
- REACH
- Regulations



Figure 2: Key goals of the REACH legislation are to characterize the risks associated with emission and exposure to specific chemicals, as well as to identify and document the conditions for manufacturing and use of the chemicals that control these risks.

The goal of the REACH initiative is that substances manufactured, imported or used in the market should not adversely affect human health or the environment. This requires members of the SIEFs to extensively test the safety of the chemicals in question and assemble the information into a chemical safety report. Part of the chemical safety report is a chemical safety assessment (CSA). The CSA is the document that assesses the following qualities of a substance:

1. The intrinsic hazards of the substances, including determination of No-Effect-Levels and concentrations as well as properties relating to persistence, bioaccumulation and toxicity.
2. The emission and exposure to humans and the environment resulting from manufacture and use of the chemical throughout its lifecycle.
3. The risks associated with emission and exposure to those chemicals.
4. The conditions for manufacturing and using the chemicals to control the risks to humans and the environment.

As comprehensive as the regulations are, there are certain exemptions that are allowed. Several major categories of chemicals are exempt because they are controlled by other European regulations. These exempt categories include pharmaceuticals, pesticides, fuels, plastic polymers and nuclear materials. One should note, however, that the chemical raw materials used to make items such as pharmaceuticals, and pesticides and the monomers used to make polymer plastics are covered by REACH. Other exempted chemicals include non-isolated intermediates, food and food additives, as well as natural substances and reaction products that fulfill certain criteria. Finally, a list of specifically exempted chemicals is maintained; e.g., glucose, water, starch, nitrogen, etc.

With such broadly reaching regulations a manufacturer, supplier, or chemical user will have to utilize a variety of analytical techniques to maintain REACH compliance. Multiple analytical tools to help companies meet their regulatory compliance are found in the Thermo Scientific molecular spectroscopy portfolio. The Antaris™ line of Fourier-transform near-infrared (FT-NIR) analyzers provides needed chemical information rapidly and reliably. NIR has many great advantages; it is a non-destructive technique, it can measure through glass and plastic containers, and it allows for remote measurements to reduce any potential hazards to the operator. The Antaris analyzers are designed to be operated by non-technical individuals and can collect data and report results safely and automatically. These analyzers use the near-infrared portion of the electromagnetic spectrum which allows for deep penetration into samples without interference from glass containers or thin plastic bags. They also offer the ability to quantify multiple components in a mixture simultaneously, negating the need to perform complex separations and multiple tests. For more in-depth chemical analysis requiring monitoring and identification of specific chemical moieties in a sample, the DXR SmartRaman spectrometer is available. This analyzer provides chemical information extremely rapidly through bottles or plastic bags and provides answers to the identity of the material using comprehensive library searches. The DXR SmartRaman spectrometer uses built-in intelligence to provide definitive sample identification without the need for the operator to have to be a Raman expert.



Figure 3: The DXR SmartRaman (left panel) and Antaris Method Development Sampling (MDS) NIR (right panel) spectrometers are valuable analytical tools for identifying, segregating and quantifying chemicals that fall under the REACH guidelines. Additionally, these tools are ideally suited to establish and continually monitor conditions for manufacture and use to limit the risks associated with the chemicals.

Near-infrared spectroscopy is a well established technology used in process control and monitoring of a great variety of materials, and is an analysis technique accepted by government and industry agencies including the United States Pharmacopeia (USP 1119); the European Pharmacopeia (Ph. Eur. 2.2.40), and ASTM (Method E 1944). Raman spectroscopy is also accepted as an analysis technique by these and other agencies (USP 1120; Ph. Eur. 2.2.48; ASTM method E1840.). Raman spectroscopy is well-established in pharmaceutical and fine chemical analytical labs worldwide and is rapidly becoming widely used in process applications.

How does the Thermo Scientific line of near-infrared and Raman instruments factor into your REACH compliance? With the daunting task looming of registering, evaluating, testing and monitoring all of the non-exempt chemicals used in your business, the Thermo Scientific molecular spectroscopic technologies can help ease the difficulties and path to compliance. Our near-infrared and Raman instruments can help in a number of capacities including:

#### Initial Chemical Identification

In order to use or test a chemical batch or lot, proper identification must be ensured. The Antaris line of NIR analyzers and the DXR SmartRaman spectrometers are designed to be used for identification of specific chemicals from commercially available or locally built libraries. Incoming chemicals and raw materials can be used directly on these analyzers without any sample preparation. This ensures more accurate identification and quantification than other methods that require more intrusive sample handling. This is particularly important when identifying chemicals that fall into the category of "Substances of Very High Concern."

#### Identification and Segregation of Exempt Chemicals

With the myriad of REACH exempt chemicals, it is important that these be clearly identified and separated from those requiring comprehensive testing and monitoring. Both lines of spectrometers can quickly separate the chemicals into groups that need further testing from those that don't. The design of the instruments and software is such that the materials can be identified by non-specialized operators directly on the process line without taking samples back to the laboratory. The identities are obtained and confirmed within seconds avoiding the time delay inherent in other techniques.

#### Concentration Determination

During the registration and evaluation phase, critical concentration data will need to be collected to determine such parameters as No-Effect-Levels for human health; No-Effect-Concentration for the environment and persistence, bioaccumulation and toxicity limits. When detection limits are appropriate, the Antaris and DXR SmartRaman spectrometer lines are instrumental in rapidly measuring and monitoring concentrations or the presence of specific chemicals from complex mixtures like biological or environmental samples. This information is required for reporting exposure scenarios. Furthermore, concentrations of multiple components in mixtures can be determined simultaneously from one spectrum.

#### Identification and Documentation of Proper Conditions for Use and Manufacture

Conditions for use and manufacture are required to be established during the initial phases of REACH compliance. Ultimately, these conditions will be part of the reported exposure scenarios. The Antaris and DXR SmartRaman analyzers are ideally suited to be placed in process environments where they can automatically monitor process conditions such as the presence and concentration of moisture starting materials, intermediates, catalysts and end-products. Additionally, human exposure and environmental emission limits can be established within the confines of the technology using these techniques. The establishment of these acceptable process conditions will eventually be a necessary part of the ongoing monitoring of exposure and emission well into the future.

#### Monitoring Accepted Chemical Emission and Exposure

Long-term monitoring will be required for chemical manufactures and end users to ensure that the established exposure scenarios and guidelines are explicitly followed. With the process monitoring capabilities of the Thermo Scientific NIR and Raman spectrometers, manufacturing facilities and chemical users will be well on their way to long term compliance with the REACH guidelines. The instruments are easy to set up and use and allow for instantaneous real-time monitoring to ensure continual compliance.

The Thermo Scientific Antaris line of NIR analyzers and DXR SmartRaman spectrometers are valuable tools for chemical manufactures and users who want to ensure their materials are REACH compliant. These tools are an integral part of rapidly identifying specific substances that are covered by the REACH legislation as well as those that are exempt. Concentrations of multiple materials can be rapidly determined simultaneously for measuring and reporting exposure scenarios. They also provide easy identification, documentation, and monitoring of proper use to determine and limit improper exposure of emission. These analytical instruments are uniquely positioned to accomplish many of the tasks required by the REACH legislation. The Thermo Scientific line of NIR and Raman spectrometers will ensure a smooth, cost effective transition to obtaining and maintaining REACH compliance.

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

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