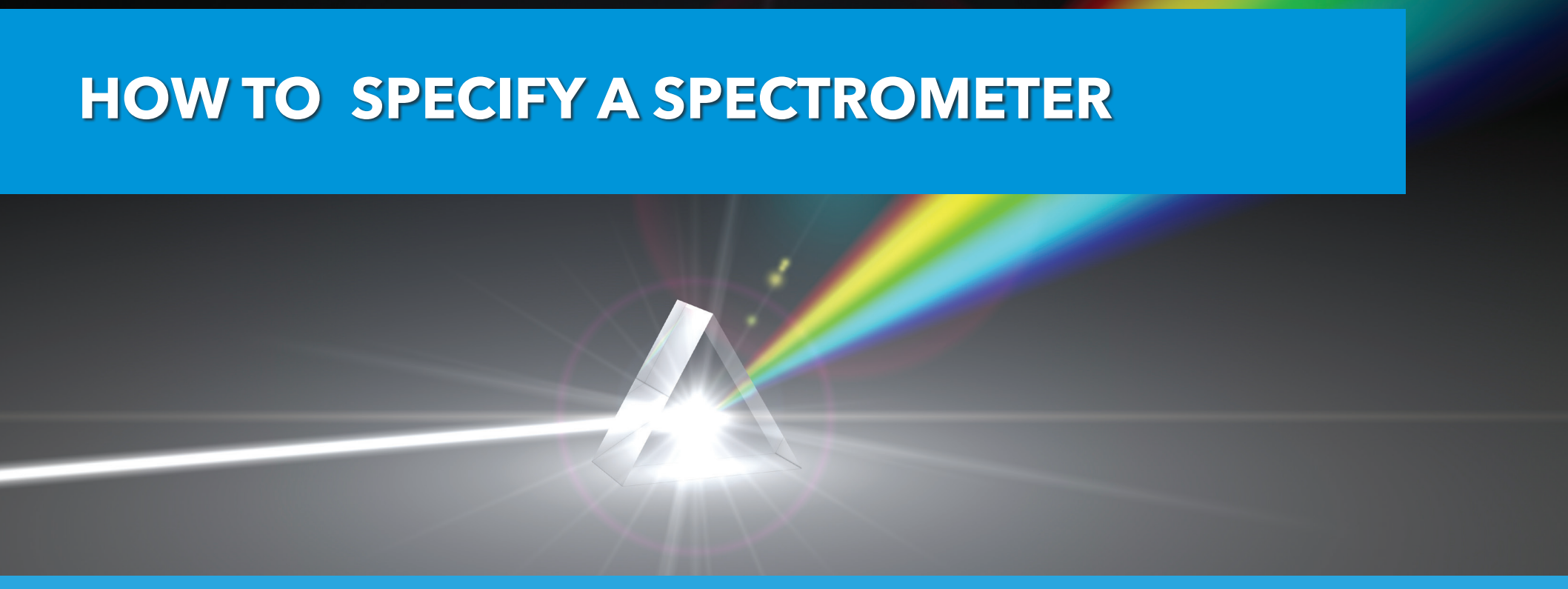
HOW TO SPECIFY A SPECTROMETER



Selecting a spectrometer is an often complicated and time-consuming process. Yet, it is highly important to be clear in what context the instrument will be used, before specifications are set. The article that follows provides some guidelines on how to come up with a proper instrument specification.

Know the application

The specification of design qualification (DQ) is highly important and often underestimated. Through the DQ, a customer can ensure that the instrument has the necessary functions and performance criteria for the application. A proper design qualification also helps to separate the important from the less important features and allows the customer to survive the "battle of features" that is often waged by instrument vendors.

In determining design requirements, it helps, if customers can specify for what application they intend to use the spectrometer. One should ask: What is the primary function or the primary problem I want solved? Do I need to test fuels for a particular material specification? Do I want to optimise my blending process or comply with government or transport regulations? Specifications should follow from those answers and reflect the user's requirements.

The design qualification also should include the answers to some very basic application-related questions. For example, will a fuel truck driver be able to measure fuel quality with the instrument? Or, will the analyzer be used by a trained spectroscopist? The requirements for various user groups will be fairly different.

Get to the core purpose

A first step in developing a specification is to get to the core purpose. Spectrometers can be used to measure many liquids, but a qualified spectrometer is already set up for a specific purpose. For example, a fuel analyzer may already be set up to measure gasoline, diesel and jet fuel, and not set up to measure waste water or solvents.

Still, an instrument may be able to measure 100+ fuel parameters right from the get go by using proven and robust fuel data from sources all around the world for analysis. But, not all of those parameters will be relevant for a particular application. Typically a limited set of parameters needs to be analyzed. So, it is important to find out if the relevant parameters are covered in the standard setup, or if a method for analyzing a new parameter needs to be added to the analyzer.

Additionally, it is important to define which type of fuels the user wants to analyze. An instrument may be able to measure finished gasolines but also test nonregular fuels like naphtha or a base gasoline without oxygenates.

Possibly, some modifications may be required to the basic analyzer setup. The instrument supplier should be able to help with setting up a dedicated naphhta database to improve results.

Specifying operation and performance

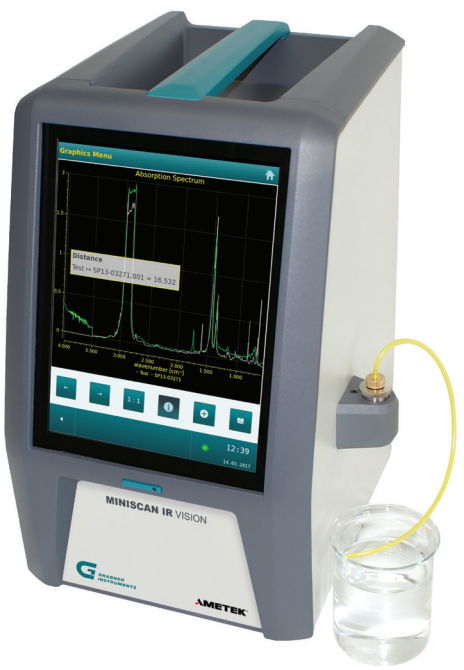
An Operational Qualification (OQ) is far more difficult to verify and specify than a design qualification. Performance criteria determine which technical aspects the instrument must fulfill to achieve the required operational performance. For example, the operation requires that an instrument uses a sample of less than 25 mL for a typical run. For the reasons of speed and accuracy, a FT-IR analyzer with an optical resolution of 4 cm-1 is required. For a good signal and reliable absorbance detection, the instrument should have a beam spliter that is made of germanium-coated potassium bromide, the cell should be made of zinc selenide, and the light source should be at least 1000°C. To quantify fatty acid methyl esters (FAME) in diesel, the instrument should use a 100 µm cell, because that is what is required to meet diesel specifications.

During OQ, performance requirements must be testable when using a calibrated instrument and traceable standards. One requirement could be to check if the instrument is able to achieve repeatability according to ASTM D5845 oxygenate specifications when 4% EtOH concentration is measured in gasoline, or if the limit of detection complies with the requirements of EN 238 benzene standard during daily analytical use.

Specify sensible criteria

As noted previously, a good specification should support the purpose for the analyzer. That includes technical specifications as well. Often, specifications look too good to be true or are not relevant to the job for which they are intended. Below are several examples of specifications that don't relate the purpose for the analyzer.

Example 1: A customer specifies a limit of detection (LOD) of 1g/L for aniline measurements for an FT-IR spectrometer that uses a 100 µm cell. The relevant goverrnment standard, however, acknowledges that spectrometers are not able to reliably



identify or quantify aniline content below 3g/L.

Example 2: Usually, when the optical resolution of a mid-infrared analyzer is discussed, the following perception prevails: The better the resolution, the better the result. But, does a resolution of 2 cm-1 have advantages over a resolution of 4 cm-1? Or, can components with similar peaks to each other be differentiated more easily (FAME and FAEE)? Another fact also holds true: The better the resolution, the higher the spectrum noise. Thus, an optimal resolution is the one that allows for a robust identification of fuel components in mid-IR spectrum that reduces baseline noise to a reasonably low level.

Specify supplier requirements

As the number of available spectrometers has increased, they have become more and more complex and, therefore, it has become more important to extend specifications to include supplier requirements.

Ideally, the instrument sales person should work as trusted advisor

to the customer and help with developing meaningful application solutions. The sales person should find out the application for the analyzer, the required performance specifications, and if an existing analyzer set up needs modification to comply with those specifications. The customer needs to know if there are limits that cannot be achieved.

The supplier should then demo the analyzer at the customer's site and run tests as well as do an IQ and OQ with the customer. Customers should ensure that the supplier can provide overall training and after sales support, answer application-related questions and do basic trouble shooting. A supplier who fulfills all of the above requirements will be in a good position to win the customer's long-term trust as well as business.

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