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• Transmission

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Effective Heated Transmission Cell Techniques for Antaris Method Development Sampling Systems

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Introduction

This technical note provides guidance for best practices in data collection when using the heated transmission cell with the Thermo Scientific Antaris[™] Method Development Sampling (MDS) FT-NIR analyzer and RESULT[™] software. Liquid samples are commonly analyzed using the transmission module; the following information offers techniques to optimize your data.

Temperature Control

Liquids are sensitive to temperature differences, and absorption peaks may shift depending on the temperature of the material. To minimize spectral differences due to temperature changes, a heated transmission cell can be used. For the Antaris MDS analyzer, the heated transmission cell will have an icon on the side as shown in Figure 1 along with a serial number for the part. Often differences in spectra are due to the variation in ambient room temperatures from day to day. To avoid this variation, the temperature

of the transmission cell can be set slightly higher than the ambient conditions (i.e., 28-30 °C). Make sure the sample and transmission cell have reached the prescribed temperature before collecting data. The time to equilibrium may be a few minutes, depending on the desired temperature.



Figure 1: lcon indicating the transmission cell is temperature controlled

Calibration Files

Each transmission cell is factory-calibrated and has calibration files (.DST files) associated with it that are stored within the Antaris. If a different heated transmission cell is used other than what has been installed in the instrument, the stored calibration files will be incorrect as will the cell temperature. Ensure that the proper heated transmission cell is being used by matching the serial numbers of the cell with those stored and displayed by the instrument. The serial number stored in the instrument is accessed through the "Instrument Status" option in RESULT Operation. Refer to Figure 2 or the Antaris Users Guide for further details.



Figure 2: Accessing the heated transmission cell serial number stored within the Antaris firmware. From RESULT Operation, click on the Maintenance tab at the top. Go to "Instrument Status"; make sure "show instrument serial numbers" is activated, and then hit OK. This will bring up a report that includes the heater block (transmission cell) serial number. Make sure the serial number of the transmission cell heater block in use is the same as that listed in the instrument report.

Use of Apertures

For most applications, the apertures included in the transmission cell should be used. Apertures limit the transmitted light to the central part of the sample vials which minimizes the influence of the cuvette walls on the spectral data. Additionally, round vials can cause "lensing" which may affect the spectrum. Figure 3 illustrates the placement of the apertures as well as the affect on the light beam.



Figure 3: The placement of the apertures as well as the affect of the apertures on the light beam is shown



Proper Background Collection

RESULT software is very flexible and can be used to collect background spectra from any position on the transmission cell. For most applications the background is collected using the automated, internal background position. The background collection is accessed by opening a Collect event in RESULT, and selecting the "Background Position" in the Background Specification window. If multiple samples are analyzed simultaneously, an internal background can be used. This is accessed in a Collect Multi-Channel event by choosing 0 under the Background Channel for individual sample channels.

Optimizing Pathlength and Gain

Aqueous solutions can be highly absorbing. This will result in attenuation of the light and large spectral peaks. Bands that exhibit absorbances greater than 3 units should not be used for quantification. Peaks that appear on the shoulders of highly absorbing bands should also be avoided. If a sample is highly absorbing, reduce the pathlength as much as possible by using narrow vials or cuvettes. Pathlengths greater than 1 millimeter should be avoided for highly absorbing samples. Change the gain and attenuation screen settings to allow for the optimal amount of light. Optimizing these settings is accomplished through the automated "Optimize Gain" feature available in a Collect event window. With the sample in place and equilibrated for temperature, activate the Optimize Gain tool to automatically determine the best screen attenuation and gain for that particular sample.

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