Determine concentrations with Paradigm workflows

TQ Analyst makes it EZ

One important application for FTIR spectroscopy is extracting valuable information about the amount of a particular component found in the sample. TQ Analyst EZ is included as part of the Thermo Scientific™ OMNIC™ Paradigm Software and provides an excellent way to create methods for obtaining quantitative measurements from the spectrum. This process can be as simple as a baseline-corrected peak area or as complex as a CLS multivariate quantitative analysis application that determines the concentrations of several components.

To demonstrate the benefits of incorporating TQ Analyst EZ methods into a workflow, we will create a simple peak height analysis based on the N-H stretching band near 3300 cm^{-1} measured on the Thermo Scientific™ Nicolet™ Summit FTIR Spectrometer configured with the Thermo Scientific™ Everest Diamond ATR Accessory. The Everest ATR Accessory with rugged single bounce diamond crystal provides a fast way to measure the amount of additive in a plastic formulation even with rigid, irregular shaped samples.

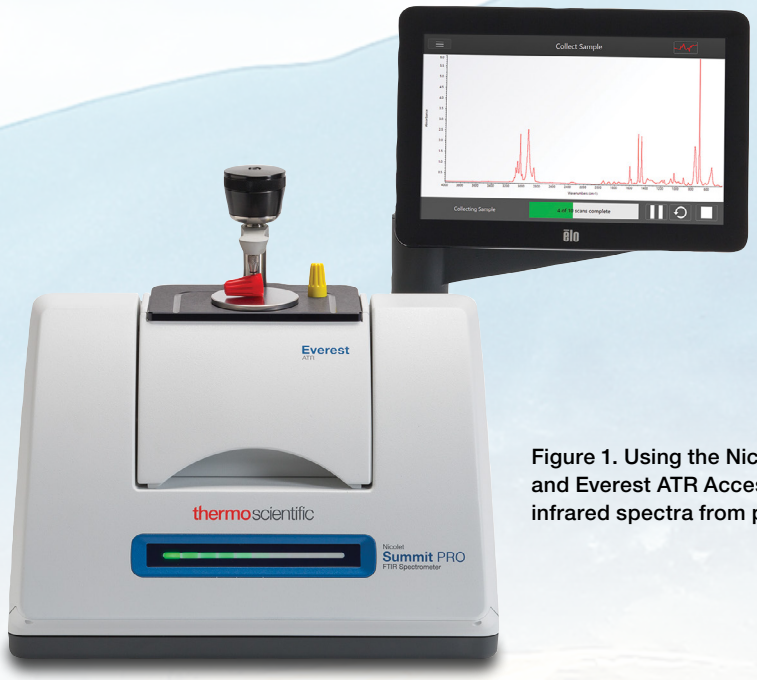

Figure 1. Using the Nicolet Summit FTIR Spectrometer and Everest ATR Accessory to acquire high-quality infrared spectra from plastic parts

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While the peak height can be measured in OMNIC Paradigm as shown below, performing this calculation in TQ Analyst EZ has several benefits when creating a workflow. The first benefit of using TQ Analyst EZ is that once the method is created, it can be used with future workflows and is also compatible with legacy OMNIC systems. This compatibility greatly reduces the risk of getting different results on different instruments. It also means that many TQ methods developed for older systems can be used directly with the instruments running OMNIC Paradigm Software.

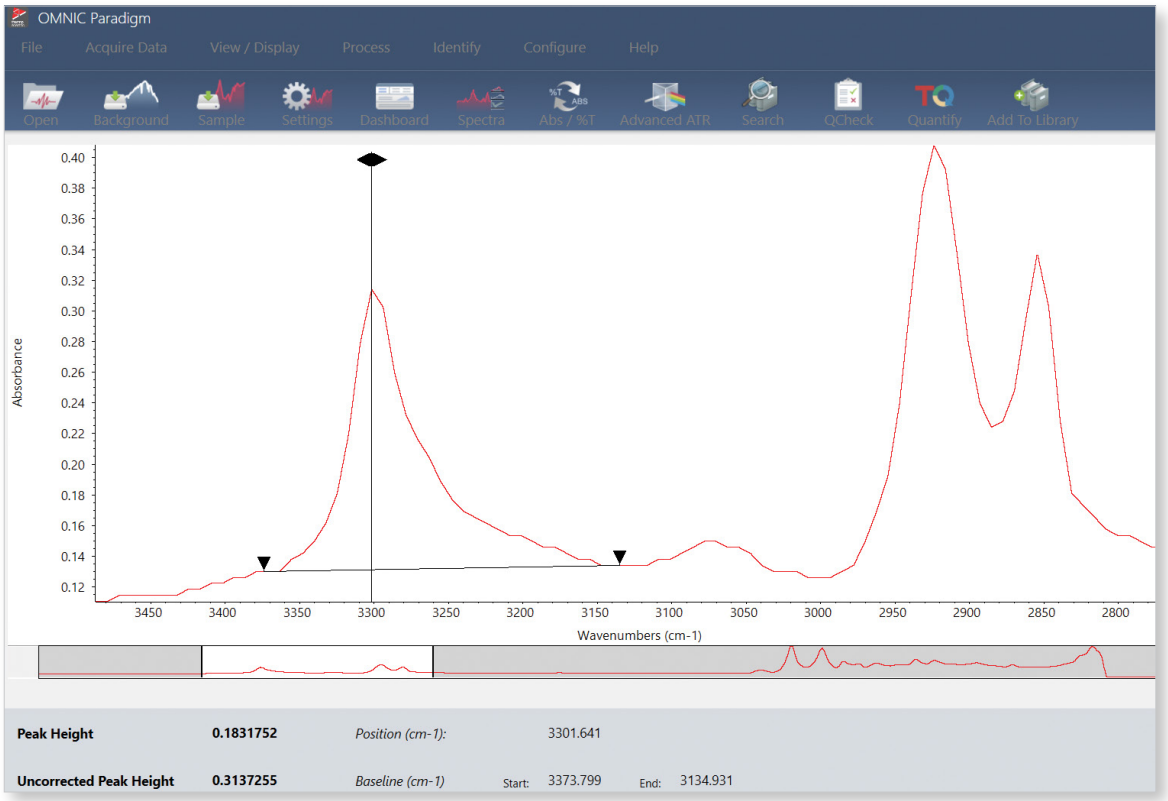

Figure 2. Measuring the N-H stretch peak height in an ATR spectrum

The figure below shows the TQ Analyst interface for creating a new method. In this example, we are using the N-H stretch peak at 3300 cm^{-1}. Assuming that Beer's law applies (Abs = A*B*C) and we know both the pathlength and the Absorptivity of this peak we can divide the measured peak height by the value to get the Concentration. In this example, we will use a Maximum Peak Height in Region with a two-point baseline to calculate the intensity of the peak.

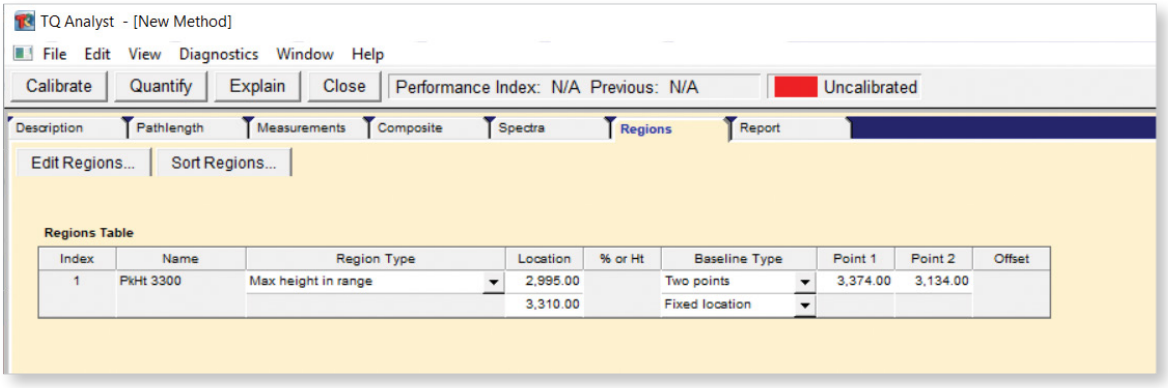

Figure 3. Creating a TQ Analyst EZ method to calculate the concentration from the peak heigth

A second benefit of using TQ Analyst EZ is the ability to create Composite Variables that can combine the values from several component measurements. Assuming the concentration is a linear function of absorbance, the Composite calculation is simple. In some cases, you may add a zero correction or even use a second-order Algebraic Formula.

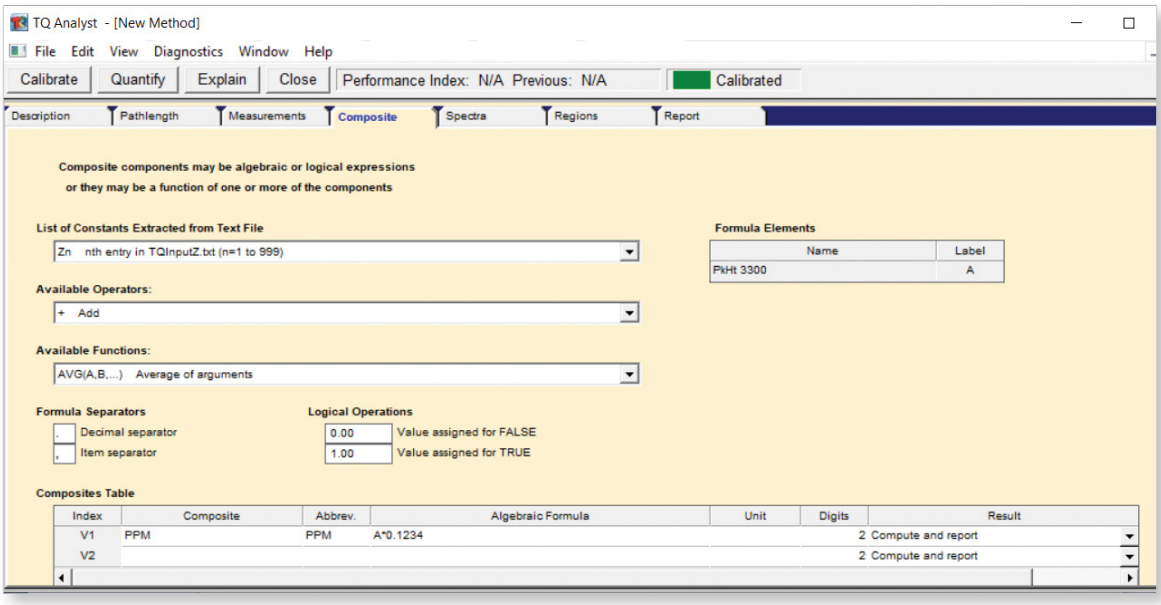

Figure 4. Using the Composite feature to scale the peak height by the absorptivity

The resulting workflow is automatically generated in the OMNIC Paradigm software. By clicking on the TQ Analyst tile, you can select the method and the spectrum you want to analyze. When the method is selected, the component names and other information are automatically displayed. In this example, the first component is the measured peak height and the second is the composite as calculated above.

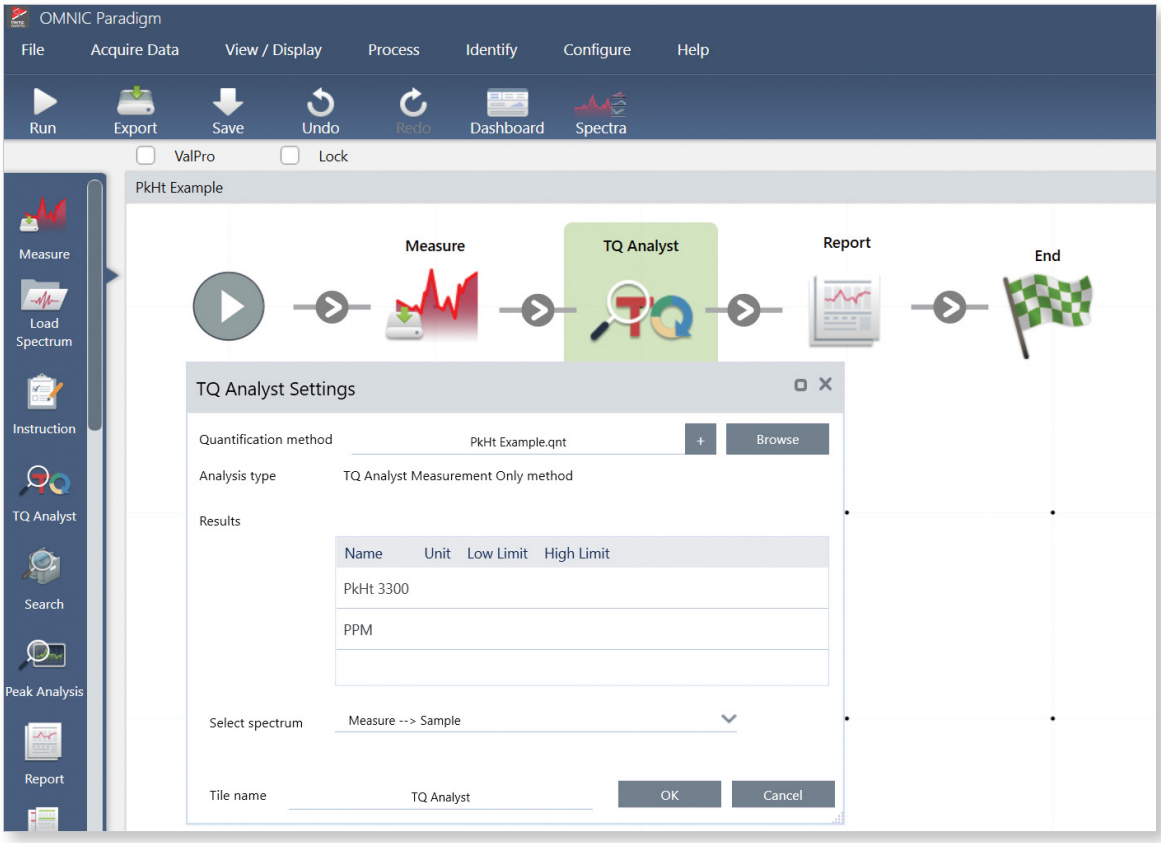

Figure 5. Adding the TQ method to a simple OMNIC Paradigm workflow

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Combining the flexibility and power of TQ Analyst EZ with the ease of OMNIC Paradigm workflow creation provides a simple way to develop an application that can be used to streamline analysis with the Nicolet Summit. For more sophisticated multi-variate analysis, TQ Analyst Professional Edition is also available.

Find out more at **thermofisher.com/summit**

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