Advantage of Collateral Data

Applied Analytics Technical Note No. 202 — Revised 19 June 2013

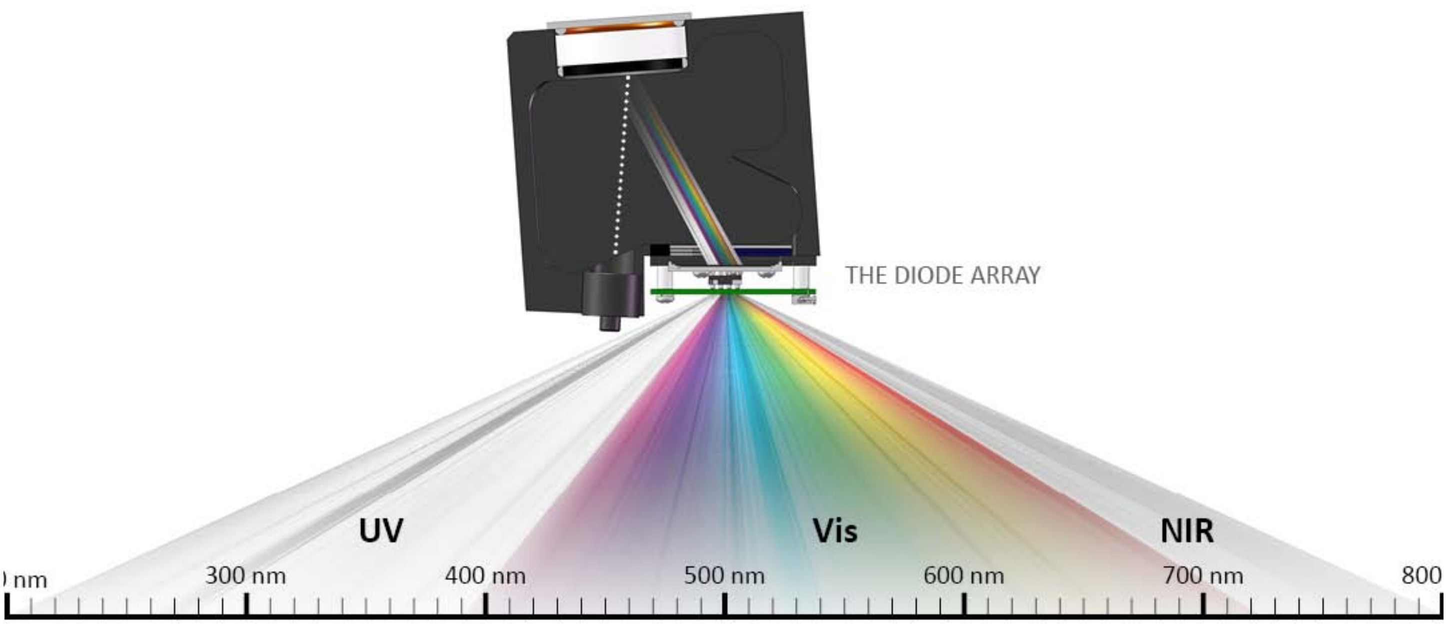
Note: this article concerns ECLIPSE for full-spectrum spectrophotometers (e.g. nova II) — not single-wavelength systems.

Dispersive 'Full-Spectrum' Analysis

'Diode array' refers to the array of 1,024 light-registering photodiodes in the spectrophotometer. Each one of these diodes is assigned by the firmware to record light at one specific energy (wavelength).

The holographic grating in the spectrophotometer serves to physically separate the received light signal into all of its constituent wavelengths, focusing each wavelength onto its corresponding photodiode within the array. This is known as 'dispersive' absorbance spectroscopy. (By contrast, 'non-dispersive' methods use filters to isolate single wavelengths and therefore destroy all data present at any other wavelength.)

Each photodiode contributes one data point to a "full spectrum" comprised of all of the data points simultaneously, ranging in wavelength from the shortest ultraviolet wavelength to the longest NIR wavelength. The actual numeric wavelength range of the spectrum is dependent on the analyzer model; most typical is the UV-Vis 200-800 nm model, which is illustrated below:



The Advantage of Collateral Data

Any single photodiode measurement is vulnerable to noise, signal saturation, or unexpected interference. This susceptibility to error makes a lone photodiode data point (as used by a photometer) an unreliable indicator of one chemical's absorbance.

As accepted in the lab community for decades, the best way to neutralize this type of error is to use collateral data in the form of 'confirmation wavelengths,' i.e. many data points at many wavelengths instead of a single wavelength. Consider the example of measuring SO_2 in a sample fluid:

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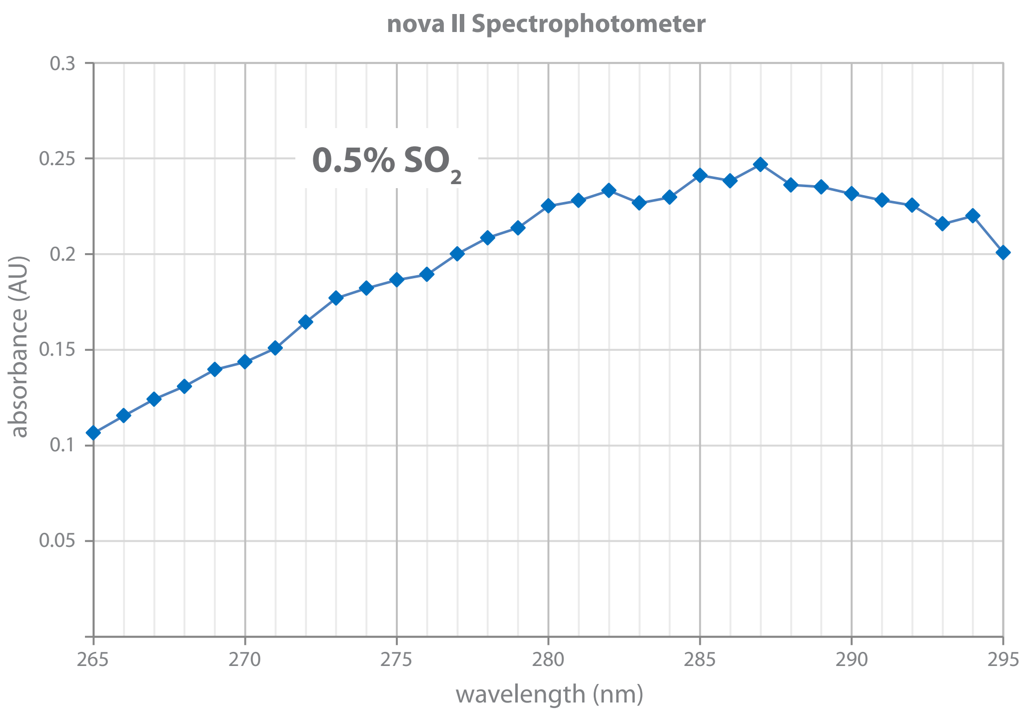

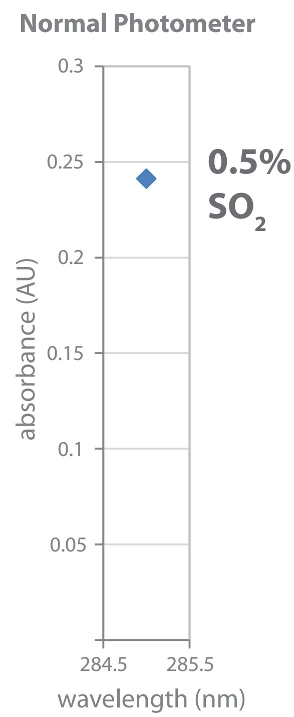

In the figures above, each diamond represents a single photodiode and data point. The nova II registers absorbance at each integer wavelength within the 265-295 nm measurement range and produces an SO_2 absorbance curve. After being calibrated on a full spectrum of pure SO_2, the spectrophotometer knows the absorbance-concentration correlation for each measurement wavelength; the system can average the modeled concentration value from each wavelength to completely eradicate the effect of noise at any single photodiode.

The spectrophotometer visualizes the SO_2 absorbance curve in this manner and knows the expected relation of each data point to the others in terms of the curve's structure. This curve analysis enables the system to automatically detect erroneous results at specific wavelengths, such as when a single photodiode is saturated with light.

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