ECLIPSE Analysis Calibration Model [ACM]

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

What is an ACM?

The analysis calibration model (ACM) — often referred to as a "Method" in ECLIPSE — is the model used to correlate chemical concentration(s) from absorbance information. The ACM tells ECLIPSE the mathematical correlation (i.e., the multiplication factor) between the measured absorbance and the real-time chemical concentration for each measured chemical.

An ACM consists of two things:

1. Calibration Standard Spectrograph

A calibration standard is an absorbance spectrum acquired while running the system on a "standard" sample of known chemical composition. This is necessary for producing the calibration coefficient (i.e. extinction coefficient), which is the correlation factor between measured absorbance and chemical concentration. This value, written as e(λ), has a precise, unique value for each wavelength in the measured spectrum.

If you were building an ACM for measuring 0-1,000 ppm H_2S, you would acquire a standard "full scale" mixture of 1,000 ppm H_2S in a similar solvent to your process background (e.g. methane, water). Running ECLIPSE on this mixture will obtain a calibration standard spectrograph of what 1,000 ppm H_2S looks like at each and every wavelength. The software divides this graph curve by 1,000 to produce the standard, or spectral building block, for 1 ppm H_2S. When running on process, the software continuously determines how many of this unit are found in the total absorbance.

2. Wavelength Range

The other setting for an ACM is the range of wavelengths that it will consider in its calculation. By looking at the distinct absorbance spectrum of a chemical, you can quickly see that there are certain regions of high structural activity (depending on the unique molecular structure) and a lot of boring, no-absorbance space. The no-absorbance space does not have any mathematical usefulness for performing this correlation (other than as a reference baseline), so we want to confine the ACM wavelength range to the region of activity including any significant peaks.

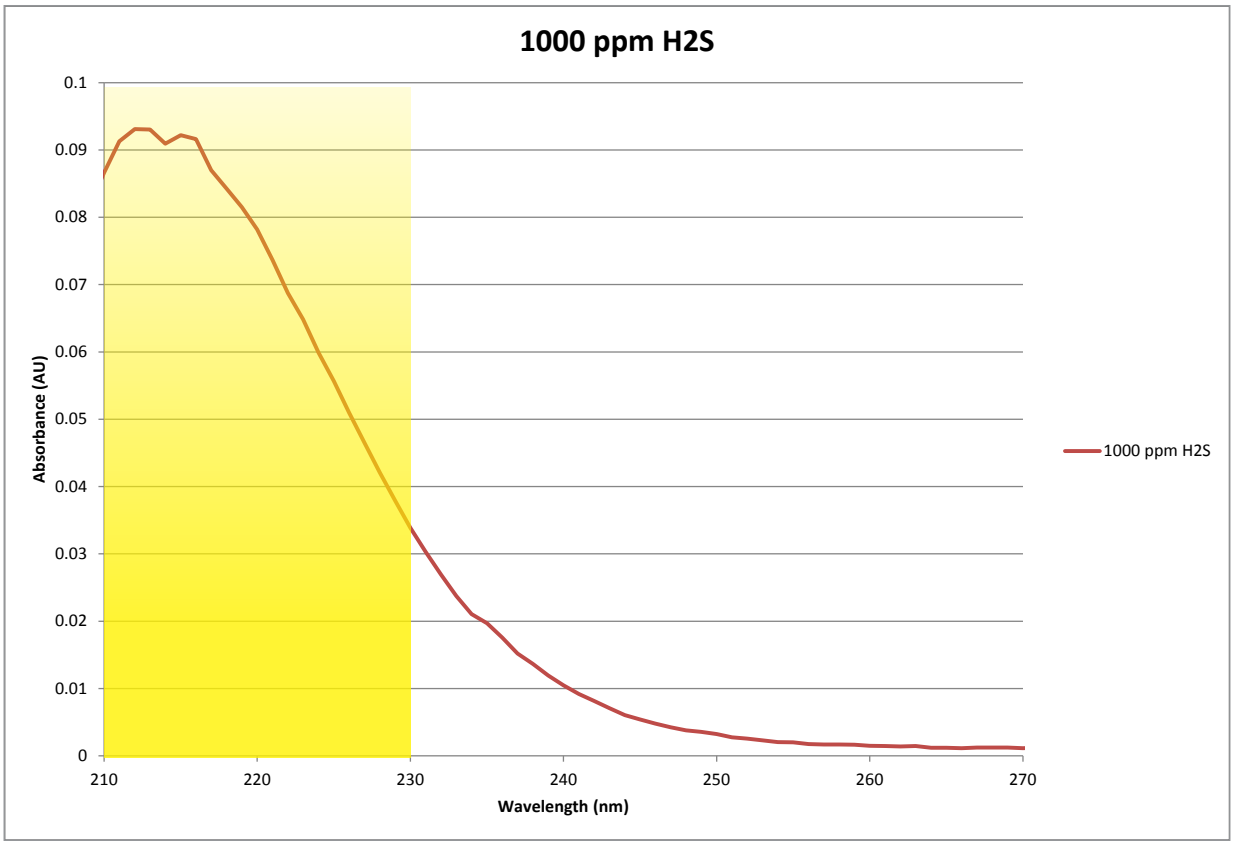
If possible, we also want to isolate a wavelength region where other stream chemicals do not absorb, so as to minimize overlapping absorbance. The software can use its DECONVOL algorithm to de-convolute overlapping absorbance, but it is ideal to have some wavelengths of single-component absorbance for perfect internal verification of the measurement.

How does using multiple ACMs establish seamless dynamic range for a spectrophotometer?

Spectrometric accuracy depends greatly on signal optimization. Each photodiode in the spectrophotometer is a light sensor that can read a saturated signal if the light intensity at its assigned wavelength is above a certain threshold. This will occur, for example, if the concentration in the process drops suddenly and the absorbance at one wavelength is much lower than the expected value, thus letting all the light through to saturate the corresponding photodiode. The reverse problem is when the sample is absorbing so strongly in the wavelength range that there is simply no light reaching the detector.

Generic multiwave photometers are locked to narrow wavelengths by optical filters and thus have limited dynamic range because of signal saturation threshold. This scenario is totally mitigated by ECLIPSE using multiple ACMs with conditional logic:

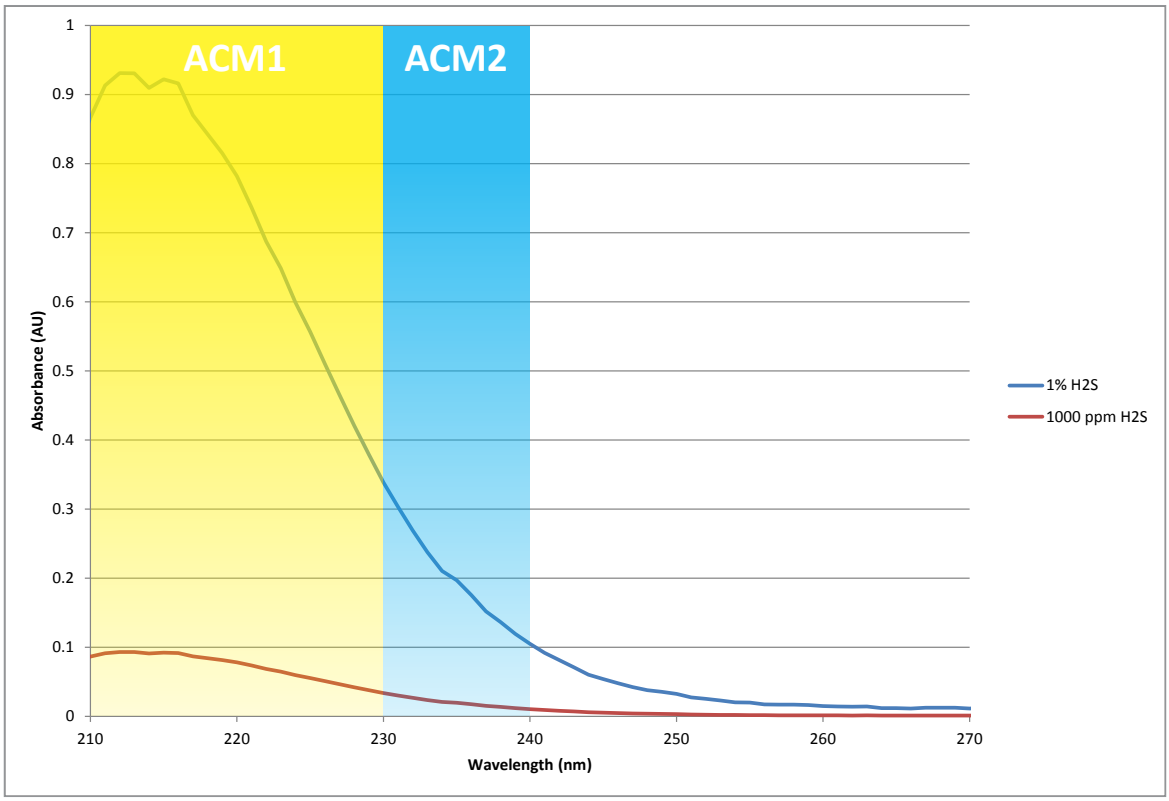
Let's say you are measuring 0-1,000 ppm H_2S. You take a calibration standard at 1000 ppm and find a good, high-absorbance region for H_2S at 210-230 nm:



ECLIPSE creates a calibration coefficient for each integer wavelength from 210 nm to 230 nm, creating 21 distinct coefficients that allow the system to recognize this absorbance curve and correlate it to H_2S concentration.

Let's say you later discover that your process fluid is spiking up to 1% H_2S, and higher! When the concentration is exceeding 1,000 ppm, you realize that the absorbance is saturated; the absorbance is so high due to the high concentration that virtually none of the light in your wavelength range emerges from the flow cell. We can resolve this situation very easily by adding a second ACM at a lower-absorbance region.

If we create ACM2 using the same calibration standard spectrograph as ACM1 but defined at the range of 230-240 nm, where H_2S absorbance is lower but still easily observable, we get 2 complementary ACMs:



Now all we need is some conditional logic to determine which ACM is read by the analog output at which time. We determine easily that if H_2S concentration exceeds 1,000 ppm, the priority ACM should switch from ACM1 to ACM2, and vice versa.

It's that easy to provide massive dynamic range using multiple ACMs. With a full spectrum at your disposal, you can do 0-10 ppm and 0-100% with the same instrument, and re-configure at any time if there are any changes to your process.

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