

Dynamic Range in Full-Spectrum Analysis

Applied Analytics Technical Note No. 204

Note: this article describes systems using full-spectrum dispersive spectrophotometers — not single-wavelength systems.

Collateral Data and Dynamic Range

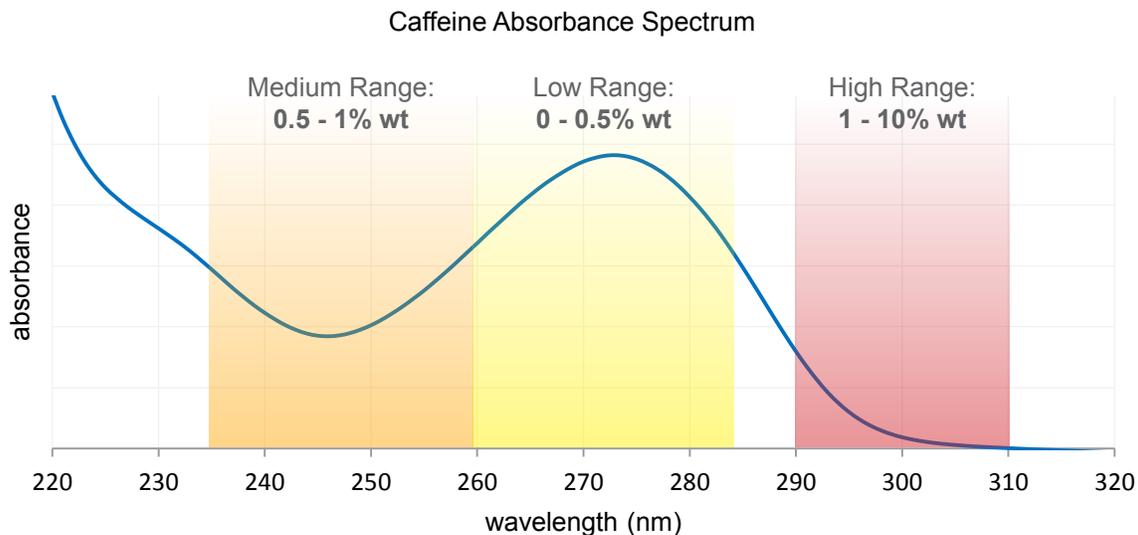
Any single photodiode measurement is vulnerable to noise, signal saturation, or unexpected interference. This susceptibility to error makes a lone photodiode data point an unreliable indicator of one chemical's absorbance.

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.

The same principle holds true for sustaining accuracy across a very wide concentration range. An instrument that only measures one wavelength at a pre-determined absorbance peak will suffer from signal clipping: above a certain concentration, all of the signal at that wavelength will be absorbed and higher concentrations cannot be measured. The full-spectrum technology used by the OMA removes this limitation by measuring at many wavelengths simultaneously.

Example: Caffeine Measurement

To illustrate this capability, the spectrum below shows the shape of the UV-Vis absorbance curve intrinsic to the caffeine molecule. Each range of caffeine concentration has a most suitable wavelength region of analysis based on the relative height of the absorbance curve within that region:



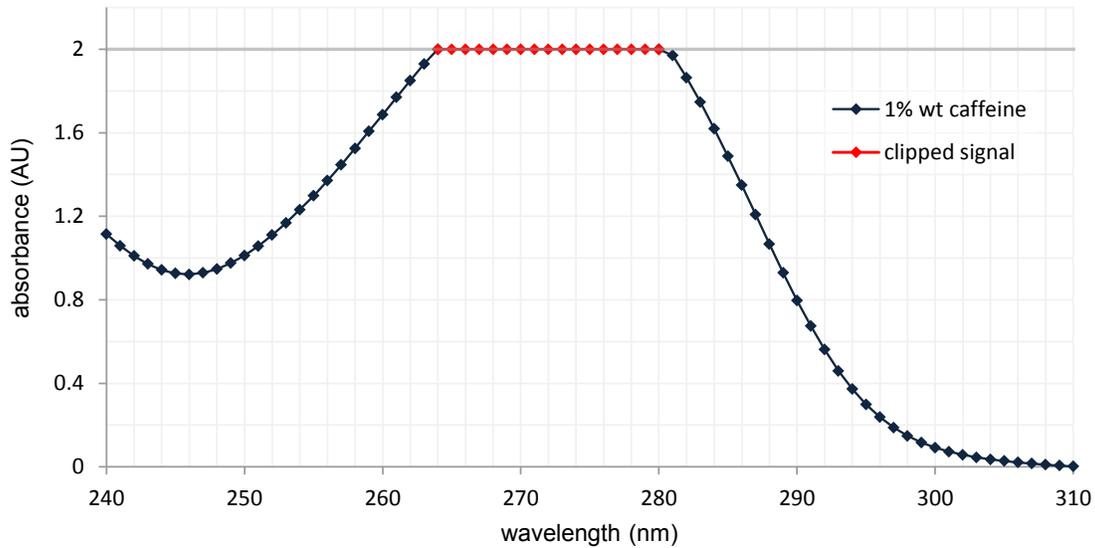
When processing the raw data from the spectrophotometer, the OMA's proprietary ECLIPSE software runs three analysis models in parallel—each assigned to a unique wavelength region—to measure caffeine concentration at different ranges. These parallel models ensure that the measurement always compensates for an error at a single photodiode due to over-absorbance or noise.

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Signal Clipping at High Absorbance

Consider the example of the Low Range: when caffeine concentration continues to rise above 0.5% wt, the sample will eventually absorb strongly enough that all of the signal in the 260-284 nm region will be absorbed and the diodes assigned to these wavelengths will register zero light intensity, as illustrated in the spectrum below:



In the figure above, the grey line represents the level of absorbance above which the photodiode will detect zero light. In effect, the signal is clipped at this absorbance and the diodes do not report accurate readings.

This graphic illustrates how absorbance clipping (a major limitation for non-dispersive photometers) is circumvented using a full-spectrum acquisition method. Even though the diodes monitoring the peak wavelengths (red) are unresponsive, the non-peak wavelength diodes (black) are still producing accurate readings. The ECLIPSE model setup determines which diodes are included in the output concentration calculation at a given concentration range.

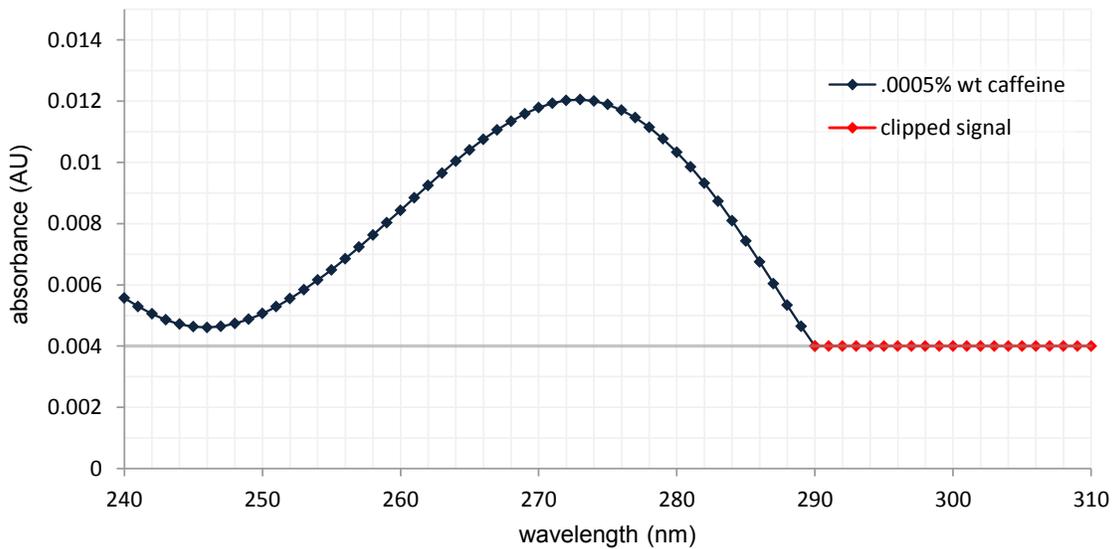
Signal Clipping at Low Absorbance

The reverse phenomenon occurs when the concentration of caffeine becomes so low that the absorbance at certain wavelengths is indistinguishable from zero. The current generation of OMA models has a photometric accuracy of ± 0.004 AU, so any absorbance below 0.004 AU can not be reliably distinguished from photometric noise.

This is illustrated in the figure below:

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In the spectrum above, the diodes reading from 290 nm to 310 nm are reading at or below the 0.004 AU threshold, so they provide unreliable readings at this level.

Wide Dynamic Range through Parallel Analysis Models

As explained earlier, Applied Analytics' proprietary ECLIPSE software circumvents these detector issues by running multiple analysis models in tandem. Each model is referred to as an 'ACM' (Analysis Calibration Model) in the software. An ACM is configured to use the measurement wavelengths which are best suited to its purpose. For example, the ACM for 0-0.5 %wt caffeine measurement is configured to use each integer wavelength from 260-284 nm.

The major benefit of this technique is that a much wider range of concentration can be accurately measured by a single solid state instrument. Within the system's defined range, there will always be one or more ACMs which can produce reliably accurate readings, and the software logic determines which values are currently reported to the user/DCS as the current output concentration.

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Further Reading

Subject	Location
Advantage of Collateral Data Technical Note	http://www.a-a-inc.com/documents/AA_TN-202_CollateralData.pdf



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