Multi-Component Analysis

Applied Analytics Technical Note No. 203

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

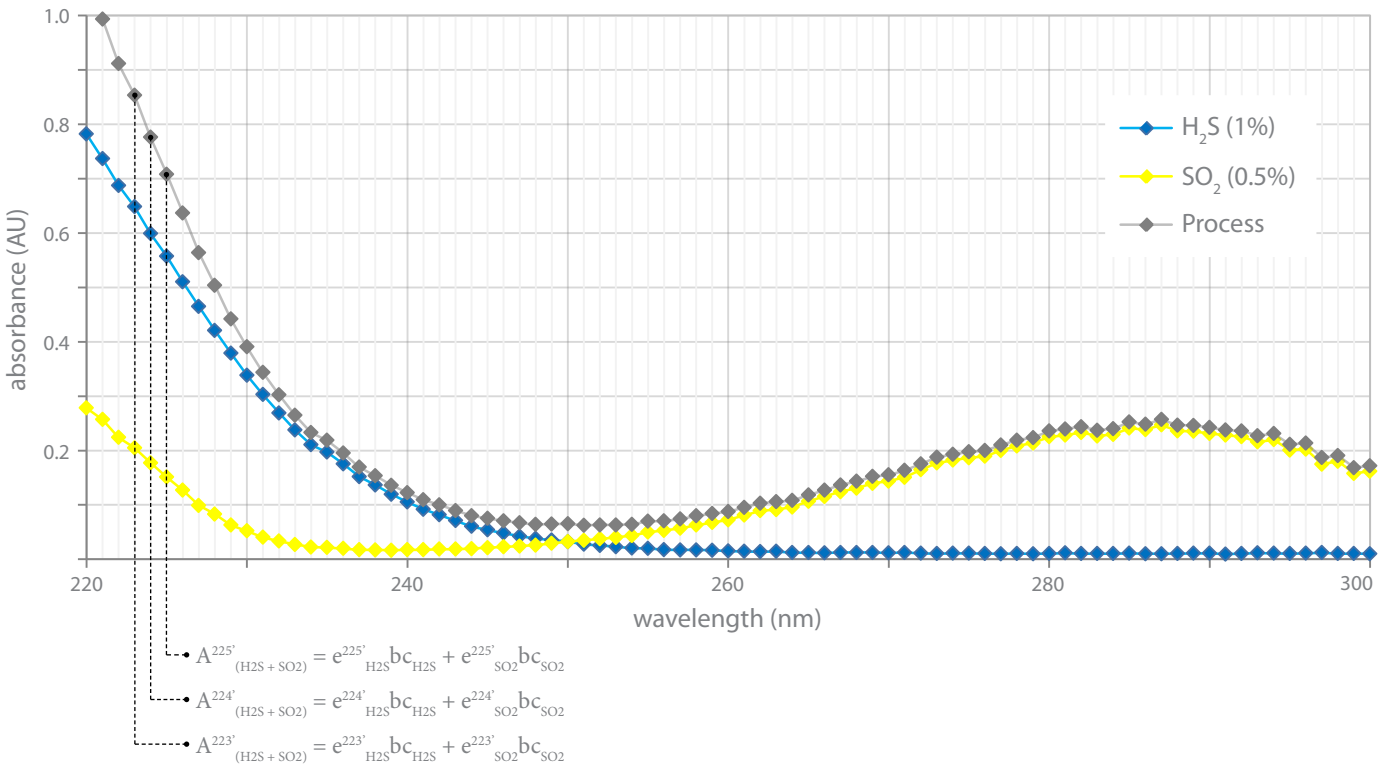
Introduction to Multi-Component Analysis

This section will explain the basic theory behind multi-component analysis performed by the ECLIPSE software.

ECLIPSE does not depend on physical wavelength isolation, moving filters, or any other data-destructive method to measure multiple analytes simultaneously. Instead, filters are applied virtually by telling the software which measurement wavelengths (i.e. photodiodes) to utilize.

All multi-component spectroscopy depends on the principle of additivity: according to Beer's law, the absorbance at any wavelength of a mixture is equal to the sum of the absorbance of each chemical in the mixture at that wavelength. A multiwave photometer measuring 2 chemicals will perform a rudimentary "2 equations, 2 unknowns" calculation using 2 measurement wavelengths to output the separate absorbance/concentration of each chemical.

With full-spectrum acquisition, a spectrophotometer uses robust collateral data and statistical averaging to perform far more accurate multi-component measurement. Consider an example of ECLIPSE measuring H_2S and SO_2 simultaneously:



As illustrated above, the ECLIPSE software uses the full spectrum to de-convolute the total sample absorbance curve and isolate each chemical's absorbance.

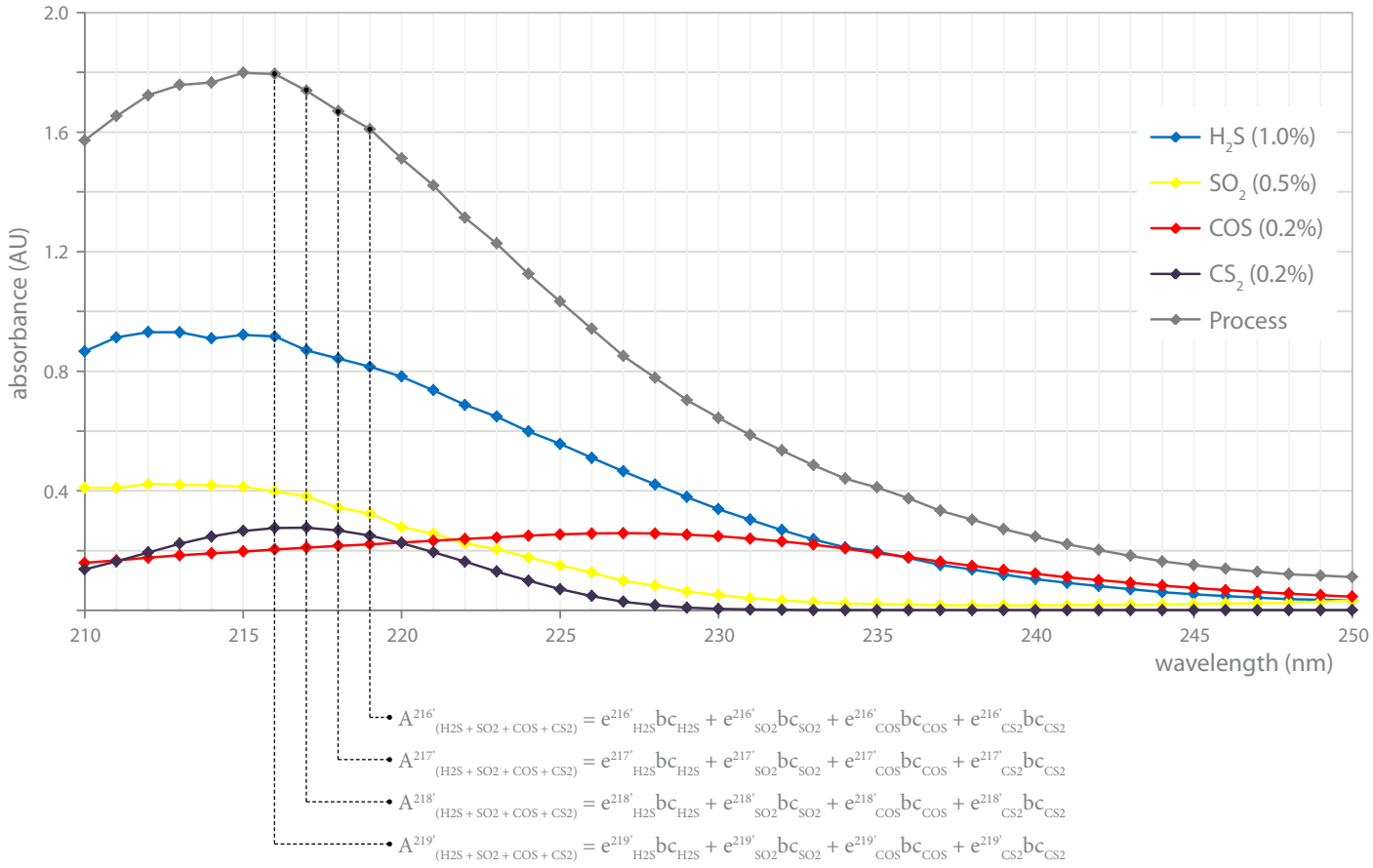
The OMA continuously solves a matrix of equations, where each equation is supplied by a single photodiode for its assigned wavelength in the form:

$$A'_{(x+y)} = A'_x + A'_y = e'_x bc_x + e'_y bc_y$$

Where *A'* is the absorbance at wavelength *', e'* is the molar absorptivity coefficient at wavelength *', c* is concentration, and *b* is the path length of the flow cell. In the image above, three such equations (for 223nm, 224nm, and 225nm) are shown. In reality, the matrix includes one equation from every single integer wavelength in the measurement wavelength range.

This robust calculation, performed with each single reading, uses the power of confirmation wavelengths and statistical averaging to achieve much higher accuracy in multi-component measurement.

To incorporate additional measurements (e.g. COS and CS_2) the OMA includes the absorbance of each compound as an additional unknown and solves a matrix of 4-variable equations:



In this analysis, we use a version of the multi-component equation modified for 4 components:

$$A'_{(w+x+y+z)} = A'_w + A'_x + A'_y + A'_z = e'_w bc_w + e'_x bc_x + e'_y bc_y + e'_z bc_z$$

where *A'* is the absorbance at wavelength *', e'* is the molar absorptivity coefficient at wavelength *', c* is concentration, and *b* is the path length of the flow cell. In the image above, four such equations (at 216nm, 217nm, 218nm, and 219nm) are shown. In reality, the matrix includes one equation from every single integer wavelength in the measurement wavelength range.

This matrix of data from many wavelengths provides far more accurate multi-component analysis within a spectral region that has heavily overlapping absorbances from each analyte.

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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