Tech Note
contrAA 800 – Background Correction

Increased robustness of the analysis by spectral background correction

Introduction

Background correction on the contrAA instrument is performed by multiple algorithms:

- Reference measurement
- Automatic baseline correction (ABC)
- Correction of spectral interferences (CSI)

ll algorithms are implemented in the operation software Aspect CS. Besides the standard procedures for ABC, the CSI tool can be applied to achieve reliable results, also for complex matrices. Once implemented into the method the selected correction algorithm is applied automatically during the measurement process.

Your Benefits

- Efficient background correction also for demanding applications
- Software-assisted correction of spectral interferences
- Independent from applied wavelength range
- Available for all atomization techniques

Background correction models in detail

Reference measurement

In general, a reference measurement without any matrix and sample is carried out by the contrAA 800 during the analysis process, e.g., with ultrapure water for aqueous solutions. Absorption bands, originating from the ambient conditions (applied gases, solvents), are detected at this step. Thus, permanent structures, which occur in the reference spectrum as well as in the sample spectrum, can be corrected automatically.

ABC - Automatic baseline correction

The correction of the baseline is performed automatically by a mathematical algorithm, called iterative baseline correction (IBC). IBC is an algorithm, which works like a high-pass filter at low frequencies. This results in sharper peak shapes of the atomic lines and a smoothing of broad background effects. At the end, a smoother baseline is obtained. The additional IBC-m mode was developed as an option especially for evaluation of molecule bands.
Alternatively, a dynamic (automatic, polynomial baseline fit) or a static (manual selection of single baseline pixels) pixel referencing algorithm can be selected.

Analytik Jena GmbH+Co.KG
Konrad-Zuse-Straße 1
07745 Jena · Germany

Phone +49 3641 77 70
Fax +49 3641 77 9279
info@analytik-jena.com
www.analytik-jena.com

Version: 08.24
NoEn

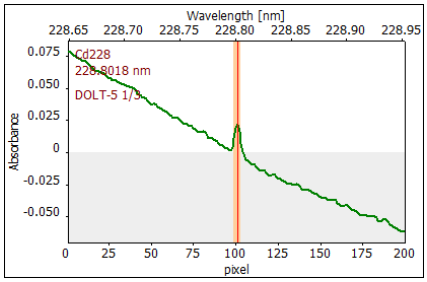


Figure 1: Spectrum without ABC

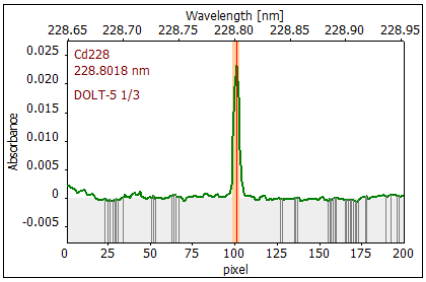


Figure 2: Dynamic pixel referencing

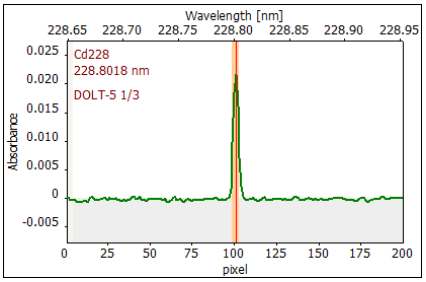


Figure 3: IBC

CSI - Correction of spectral interferences

Reagents for sample preparation and complex matrices components may cause spectral interferences by atomic and molecule absorption, resulting in spectra with partial or direct overlapping of the analyte peak. Thus, measurement results can be falsified.

Using the mathematical algorithm tool Least Squares Background Correction (LSBC), these interferences can be compensated. LSBC is a mathematical procedure, making a linear fit of one or more pre-recorded reference spectra to every single sample spectrum. Finally, the reference spectrum is subtracted from the sample spectrum to eliminate or even eliminate the overlaying pattern.
The line identification database, which is integrated in the Aspect CS software, gives an indication about possible interfering atomic lines and molecule bands in the spectral observation range around and at the analysis line (Figures 4-5).

No.	Molecule	Factor	Offset
1	CS	1	0
2	OH	1	0
3	PO	1	0.005
4	SiO	1	0

Figure 4: Spectral database, providing a list of possible interfering molecules

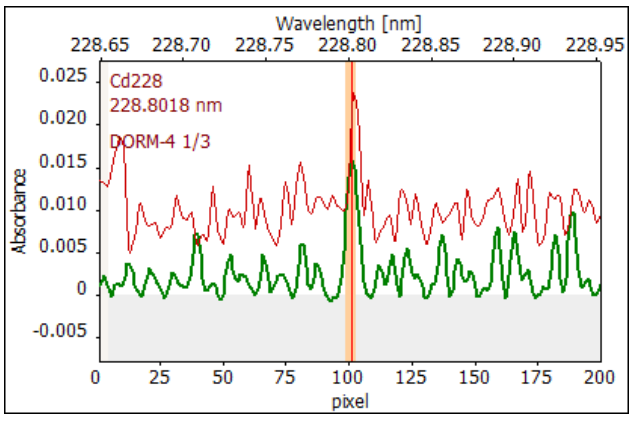


Figure 5: Original sample spectrum (green) and selected comparison PO spectrum (red) from the spectral molecule database

Solutions containing the identified matrix components causing the spectral overlay, are measured using the applied method parameters (Figure 6). The resulting matrix spectra are used for the correction of the spectral interferences. The software detects the relation between all single molecule bands, appearing in the observation range. Since any change in concentration is going to affect all molecule bands by the same

Analytik Jena GmbH+Co.KG
Konrad-Zuse-Straße 1
07745 Jena · Germany

Phone +49 3641 77 70
Fax +49 3641 77 9279
info@analytik-jena.com
www.analytik-jena.com

Version: 08.24
NoEn

factor, the concentrations of the matrix components do not have to match exactly the concentration in the samples.

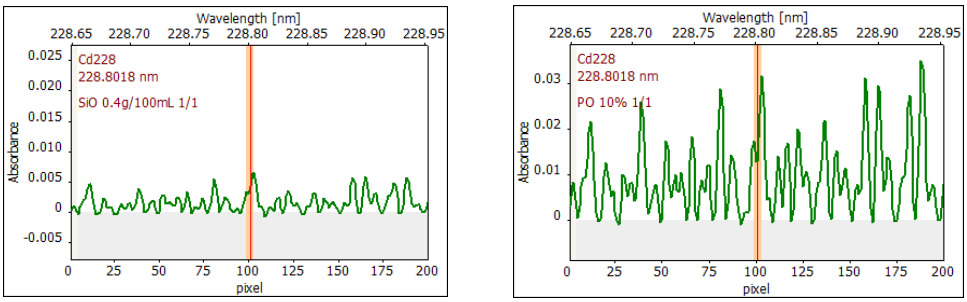
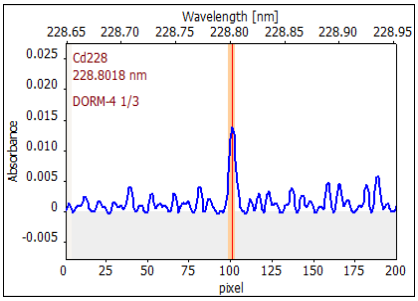
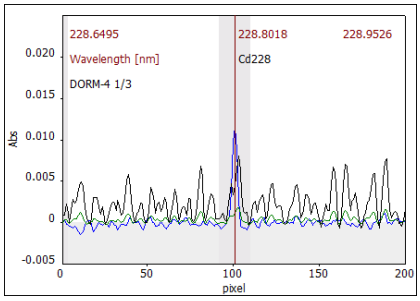
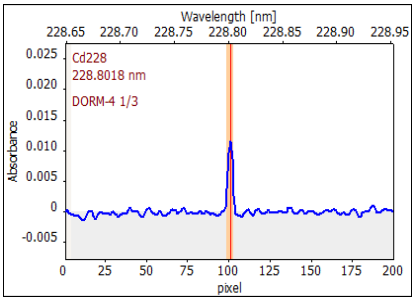


Figure 6: Correction spectra of SiO (left, recorded by using a suspension of 0.4g SiO_2 in 100 mL deion. H_2O) and PO (right, recorded by using a 10 % $NH_4H_2PO_4$ solution)

Up to five individual recorded correction spectra can be combined to a correction model, which is subsequently integrated into the analysis method.

Table 1 shows the effect of a created correction model on the analyte peak and the baseline.

Table 1: Example for recorded correction spectra and correction model for CSI for the determination of Cd in soil certified reference material (CRM)

Sample spectrum without correction	Recorded correction spectra	Corrected sample spectrum
		
	Display of a correction model, containing all applied single correction spectra (blue: corrected sample spectrum, green and **black**: correction spectra of SiO and PO)	Certified concentration CRM: 0.299mg/kg
		Measured concentration of CRM: 0.304mg/kg

Analytik Jena GmbH+Co.KG
Konrad-Zuse-Straße 1
07745 Jena · Germany

Phone +49 3641 77 70
Fax +49 3641 77 9279
info@analytik-jena.com
www.analytik-jena.com

Version: 08.24
NoEn

Tech Note
contrAA 800 – Background Correction

Summary

This unique feature of the contrAA 800 is based on the high-resolution continuum source technique, where a spectral section is detected. The spectrum provides information beyond a single element line and offers many advantages in data evaluation. If required, other elements contained in the sample, which occur within the spectral observation range can be quantified simultaneously. Thanks to the various options for background correction, interference can be easily detected and reduced or even eliminated, and the resulting analyte signal can be evaluated without a recognizable interference influence. The 2D and 3D spectral display illustrates the interferences that are not plottable in the conventional line source AAS, and the used mathematical algorithms can be visually tracked.

The ASpect CS software gives the opportunity to customize the evaluation of the absorption signal using the automatic baseline correction (ABC) and simultaneous correction of spectral interferences (CSI) to ensure correct results, even for challenging samples with high matrix load.

Reference: TechNote_AAS_0003_en.docx

Analytik Jena GmbH+Co.KG
Konrad-Zuse-Straße 1
07745 Jena · Germany

Phone +49 3641 77 70
Fax +49 3641 77 9279
info@analytik-jena.com
www.analytik-jena.com

Version: 08.24
NoEn