Differences Between EasyCal and SpectraEDX: An Overview

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Calculation Methods and Other Differences

EasyCal:

- Uses Lucas-Tooth intensity-based calculation
- One-pass, non-iterative
- Line library fixed, uses gross or net intensity
- Preparation fixed
- Completely empirical
- Single phase only
- Modules are enabled

SpectraEDX:

- Uses LaChance or Fundamental Parameters-based calculation
- Iterative calculations
- Line library can be defined by user
- Preparation can be defined by user
- Partial to full empirical, chosen by user
- Multiple phases possible
- Modules are not supported

Fundamental Parameter Method

Matrix corrections (absorption and enhancement) based on concentrations can be calculated from fundamental parameters, but details of spectral distributions and instrumental geometry are divided out by referencing all intensities to those of pure element standards.

That allows the concentrations to be calculated as ratios of the measured intensities to the matrix corrected intensities from a pure standard.

$$C_{iu} = \frac{I_i}{I_{pure}}\left[1 + \sum_j^N a_{ij}C_j + \sum_j^N e_{ij}C_j\right] = R_i\left[1 + \sum_j^N m_{ij}C_j\right]$$

Fundamental Parameter Coefficients

$$\begin{bmatrix} C_1 \\ C_2 \\ . \\ . \\ . \\ C_N \end{bmatrix} = \begin{bmatrix} 1 & m_2 C_2 & . & . & m_{N1} C_N \\ m_1 C_2 & 1 & & & . \\ . & & . & & . \\ . & & & . & . \\ m_{1N} C_N & . & . & . & 1 \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \\ . \\ . \\ . \\ R_N \end{bmatrix}$$

1. Initial C_i's are estimated (without corrections) and normalized to 100%
2. Use concentration estimates to calculate m_{ij}'s from fundamental parameters.
3. Recalculate C_i's and renormalize to 100%.
4. Repeated until convergence is achieved.

LaChance–Traill: Concentration-based calculation

Calculation method of SpectraEDX empirical alphas

$$C_i = R_i\left[1+\sum_{j}^{N}\alpha_{ij}C_j\right]$$

Concentration on both sides: iterative method

For unknown ratio of I/I_{pure} → $R_i=B_i+K_iI_i$

Lucas–Tooth: Intensity-based calculation

Calculation method of EasyCal

$$C_i = K_i I_i \left[1 + \sum_j^N \alpha^*_{ij} I_j \right]$$

Intensity on this side: single pass calculation

Empirical Calibrations

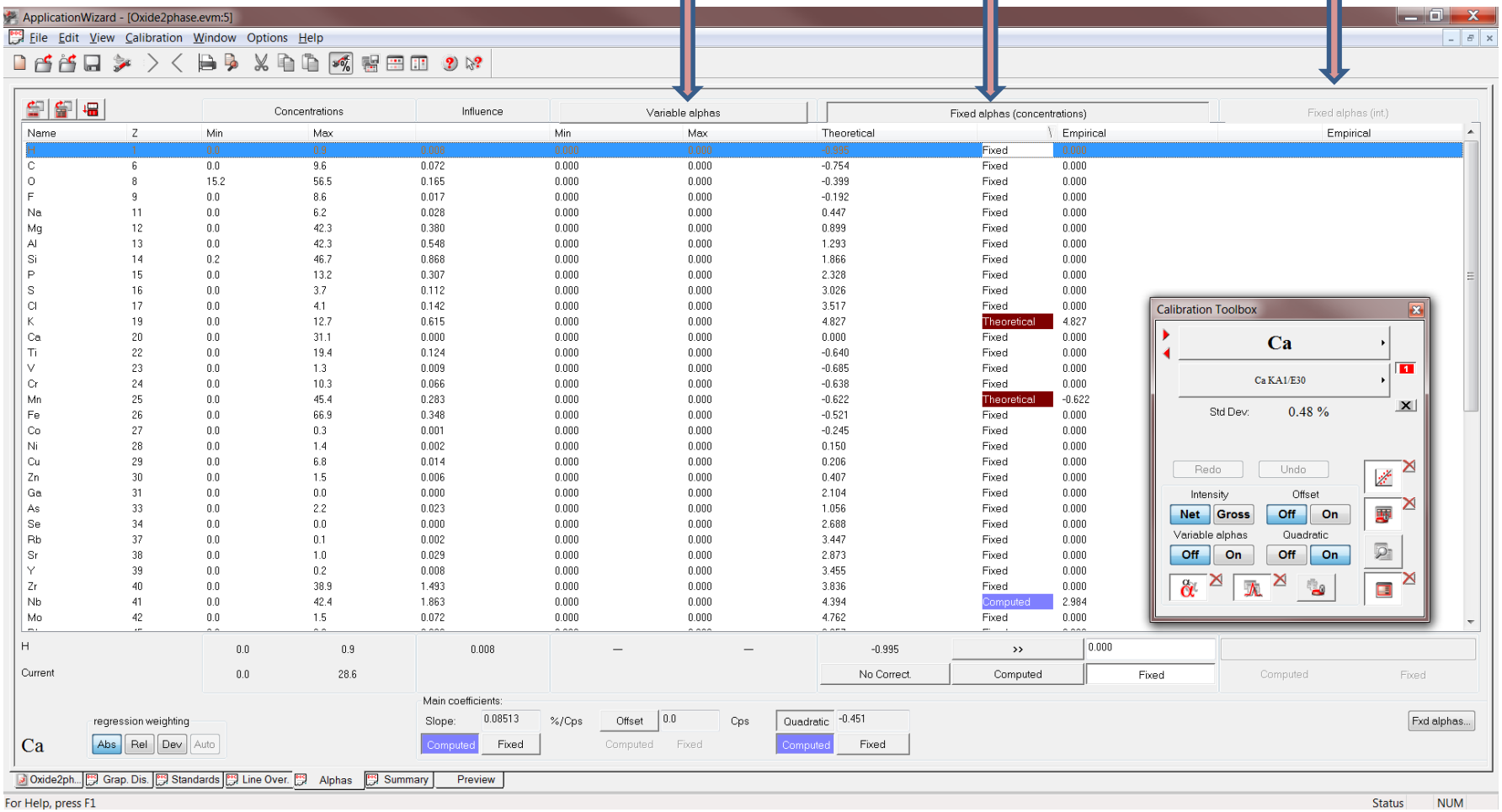
- The α_{ij}'s are simply the "best fit" values and must be determined from a suite of reference materials without concentration correlations.
- It is up to the calibrator to edit the matrix of αs to make sure the correlations are physically reasonable.
- Empirical method can be used only within the concentration ranges covered by the calibration.
- Empirical method is not applicable if there are any fundamental differences in sample form, instrumental geometry or measuring conditions.

Different Methods in SpectraEDX

Fundamental Parameters (only in full SpectraEDX)

LaChance (only in full SpectraEDX)

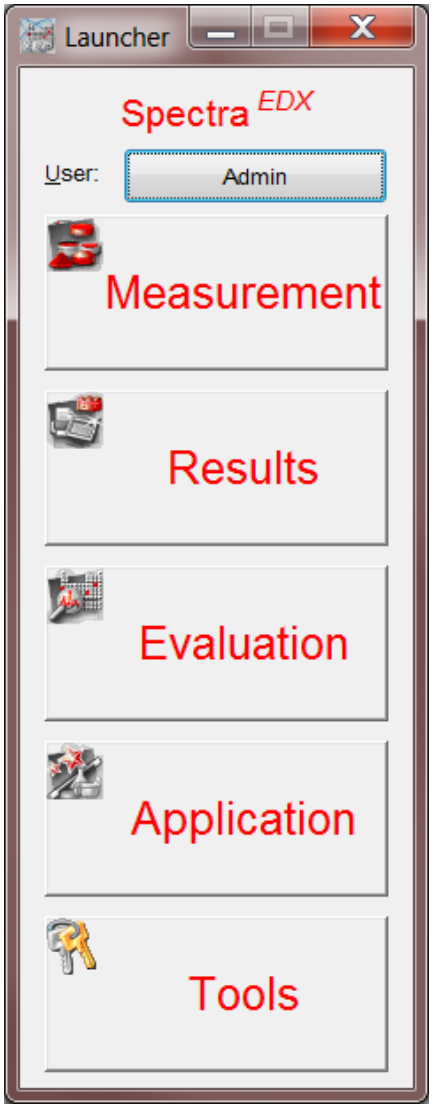
Lucas-Tooth (only in EasyCal)

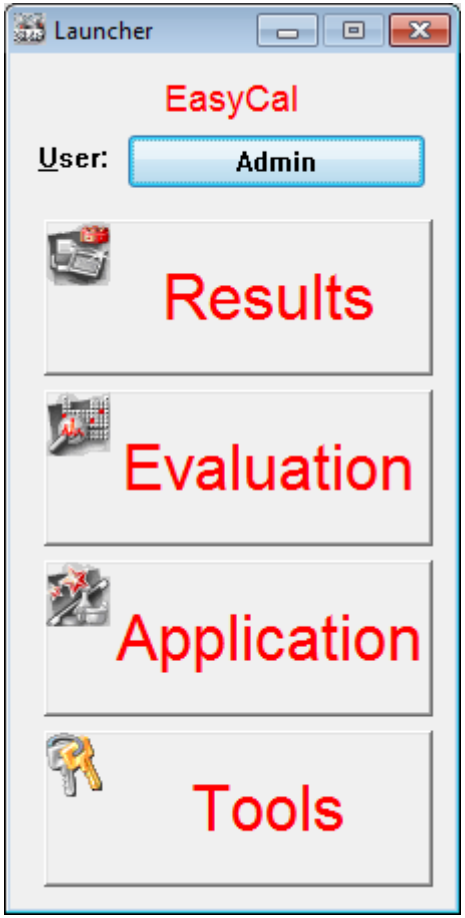


Visual Differences

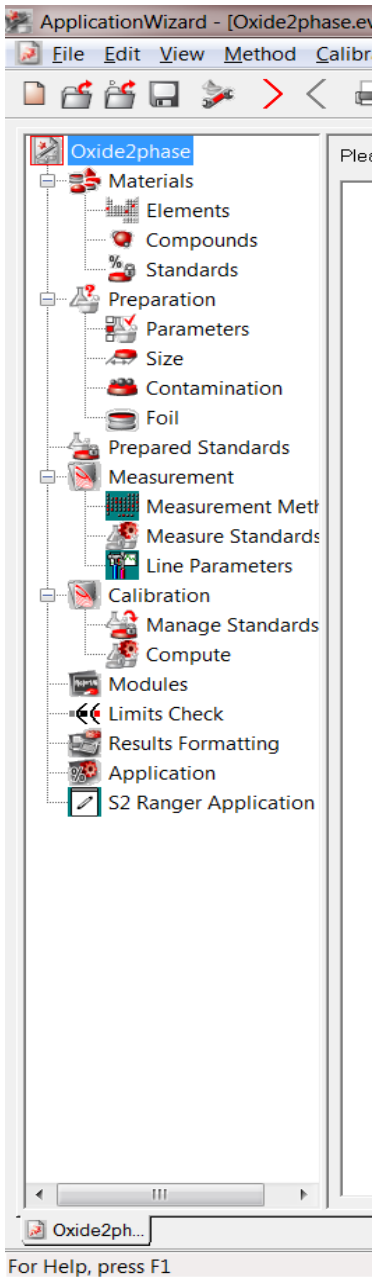
Launcher

(I said “lunch” not “launch”...)



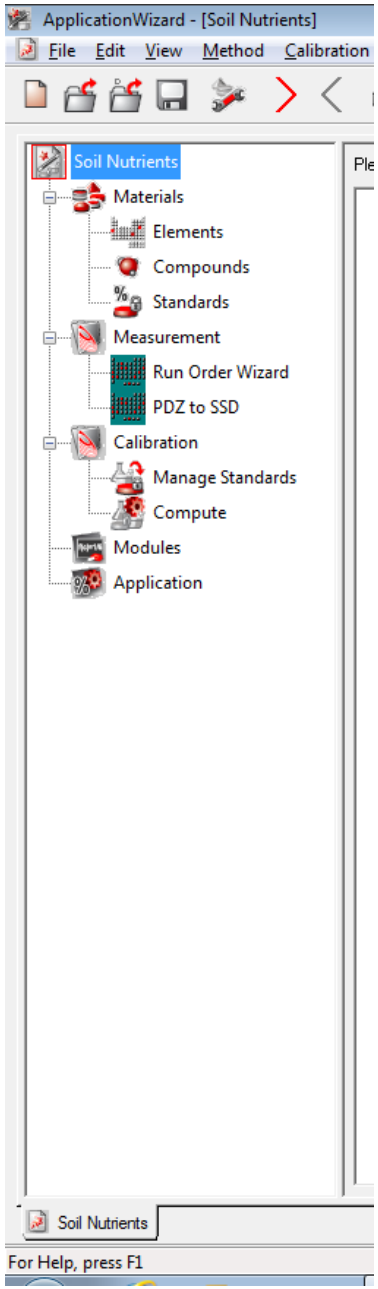


Menu Structure

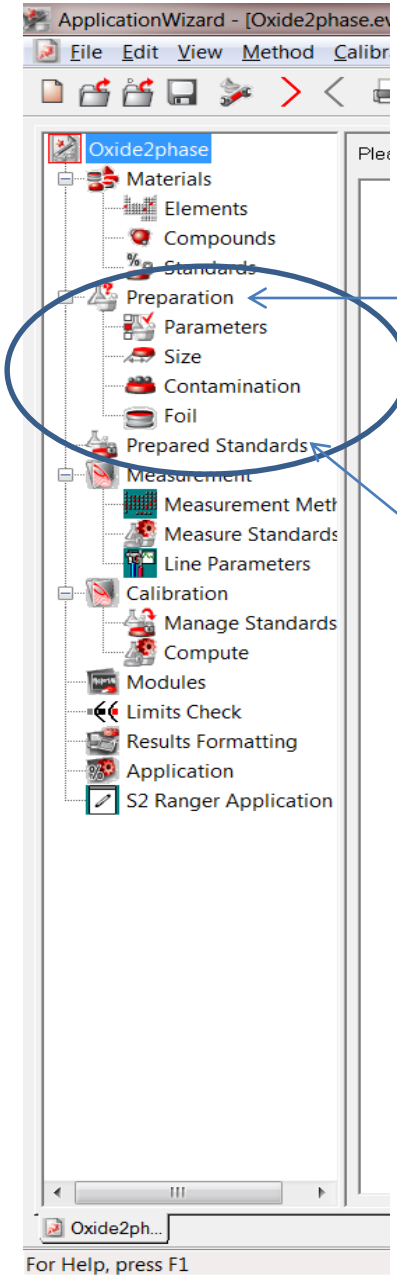


SpectraEDX

EasyCal



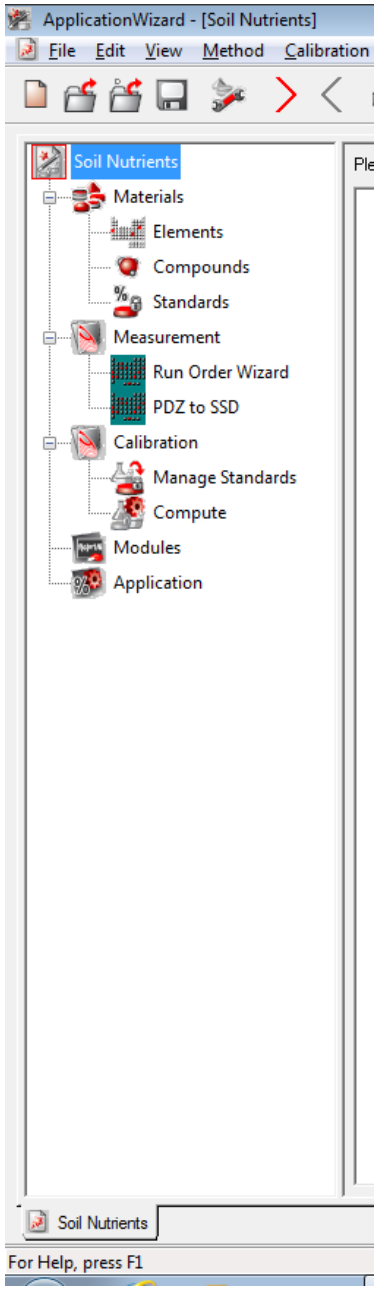
Preparation



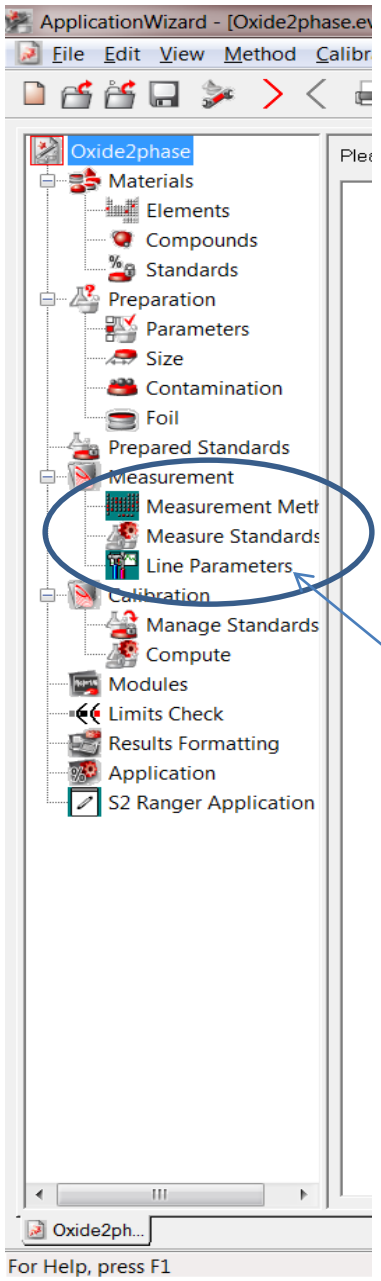
In SpectraEDX, the user creates a preparation, including any binder or foil used in the standard.

From the defined material, a set of prepared standards is chosen to be used in the calibration

In EasyCal, this section is missing. The preparation is automatically created by the software. All samples are assumed to be solids and all samples defined in the material are used in the preparation.



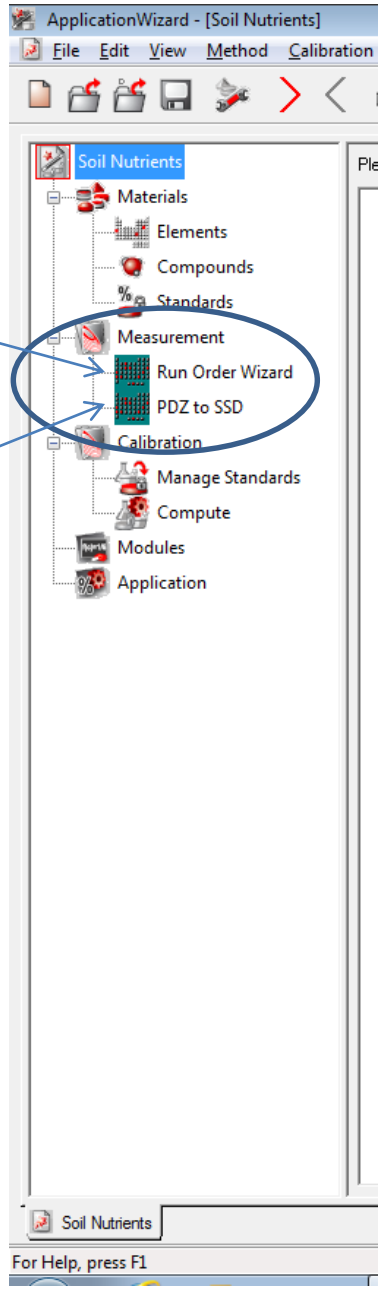
Standards Measurement and Line Library



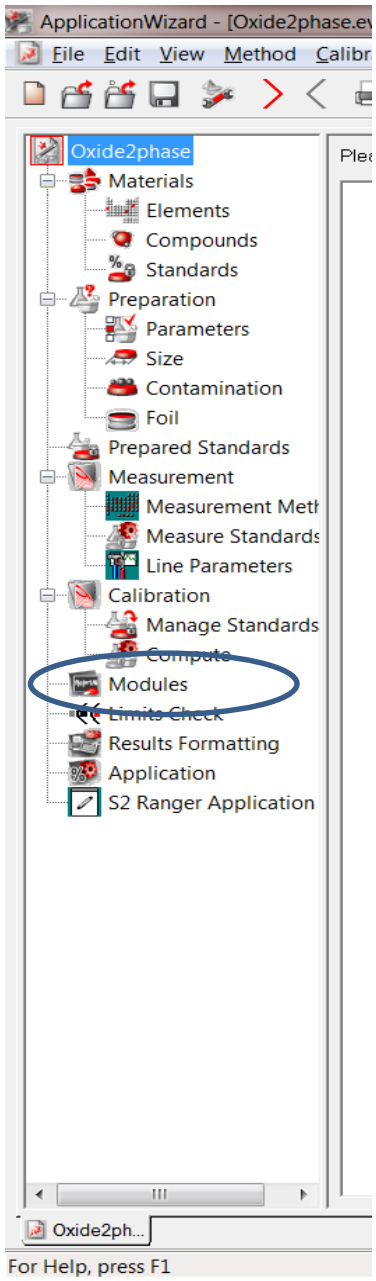
In EasyCal, the software creates a run order to use in measuring the calibration standards.
The measured standards (pdz files) are converted using the PDZ to SSD tab.

In SpectraEDX, this section is used to define and edit the line library. The user must create his own run order csv file and use Caltoolkit to do the pdz to ssd conversion.

In EasyCal, the line library is automatically created and only uses lines for elements defined in the Materials section.

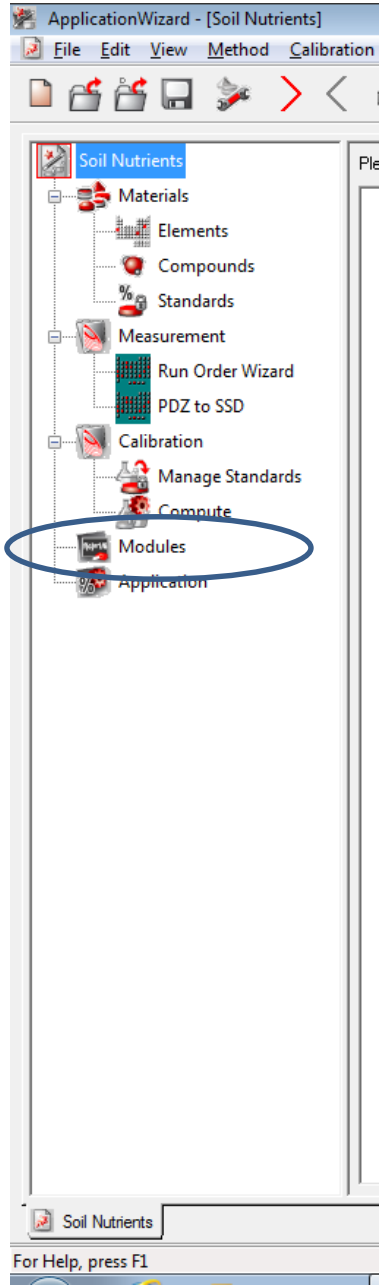


Modules

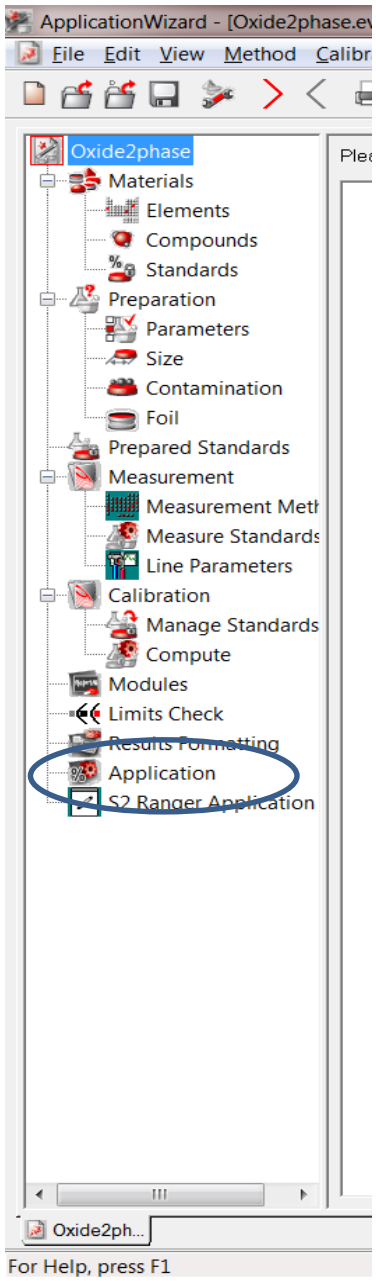


Although Modules are available in SpectraEDX, they are not supported on the instrument. They are supported for EasyCal on the instrument.

Modules defined in EasyCal are automatically incorporated when the application is saved. The module results are reported on the screen of the instrument and in the Results.csv file. If normalization is used, the module results are **not** included in the normalization.

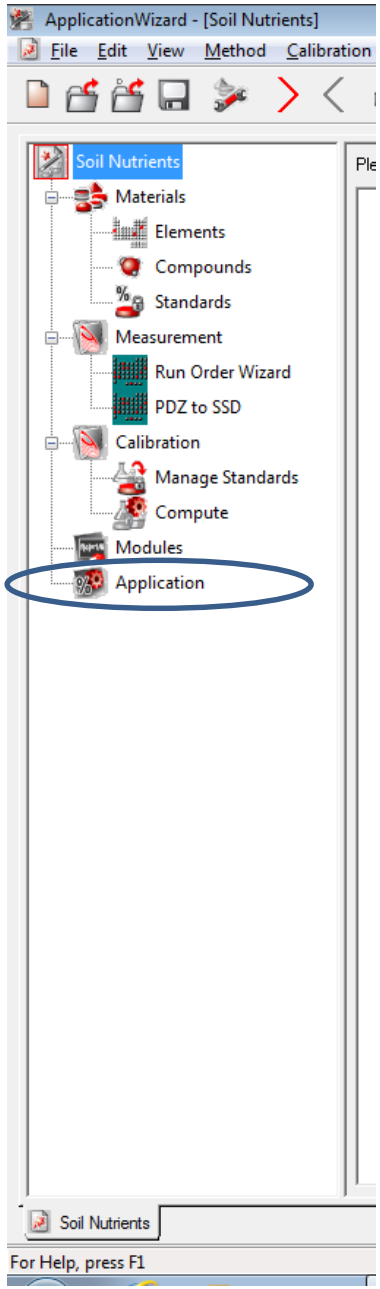


Saving the Application



In EasyCal, after creating and editing an Application, saving the application will create an install file that can be loaded directly on the instrument in the Packages folder. The file will create all necessary folders as well as an aen file, calibration file, and line library.

In SpectraEDX, the user must create and edit the application, save it, create a calibration file, and then manually create the aen and convert the line library from fll to xrd. These files can be copied to the instrument through BIT. The file folder needs to be created manually in the TitanCals folder.



When to Use Which Program

EasyCal should be used when:

- The user is not familiar with using full SpectraEDX,
  AND/**OR**
- A single type of matrix is being used for all samples
- Only a single phase is needed
- The calibration samples cover the ranges to be measured
- A calibration is desired that is quick and easy to load on the instrument
- Modules are needed

Full SpectraEDX should be used when:

- The user is familiar with using full SpectraEDX,
  AND one or more of the following are true:
- Multiple matrix types are being combined
- Multiple phases are needed
- Some FP-based theoretical calculations will be used
- Preparations are important
- Manipulation of the line library parameters is necessary
- Full control over matrix corrections and overlaps is needed

Why Can't EasyCal Allow Multiple Phases?

(We have been asked this question repeatedly)

EasyCal was developed because

- S1CalProcess is no longer supported by Microsoft software
- It is too hard to train most customers to use SpectraEDX

It is NOT designed to allow full capability for all calibration needs

If EasyCal included multiple phases, it would no longer be easy to use and to train customers to use

Multiple phases can be done by creating multiple EasyCal calibrations and doing separate measurements (that's what was done with S1CalProcess)