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**UThProcessor v2.0.2**

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This function determines U and Th isotope ratios (229Th/230Th, 236U/234U, 235U/234U) in sediment/sea water digests based on raw count files obtained by ICP-MS. The following processing steps are undertaken (in this order):

1. Tailing correction (only 230Th raw counts and sediment digests)
2. Blank correction
3. Averaging raw counts over submasses and analysis runs
4. Calculating isotope ratios
5. Mass bias correction

Optionally, further processing steps can be undertaken to determine 230Th and 234U concentrations (isotopic dilution) as well as preserved vertical particle fluxes (230Th-normalisation). Those steps require extra data input.

**INITIAL CONDITIONS**

In order to perform the blank correction, this function reconstructs the sequence of sample, blank (ICP-MS acid wash) and standard (natural uranium) measurements performed during the analysis. In order for the sequence to be generated correctly it is important that following conditions are met:

1. Only **one analysis sequence** can be processed **at a time.**
2. Sample, blank and standard raw **file names** each need to have a **unique character sequence**, e.g.
   * samples: analyst's initials or "Sample"
   * blanks: "Blank" (default)
   * standards: "NatU" (default)

Note: If no unique character sequence exists, one needs to be added to the file name!

1. All **raw files** need to be placed **in one folder**.
2. The **alphabetical order** of sample, blank and standard files as listed in the raw data folder needs to be **concurrent with the chronological order** of their analysis. Pay particular attention to the position of the sample standard and procedural blank. Keep in mind, that Matlab sorts alphabetical characters after numerical ones, which may differ from the operating system's sorting (MacOS places alphabetical characters before numerical ones, see *example\_file\_list.png* for an example of a suitable file list).
3. The analysis sequence needs to start as follows:

**Blank - NatU - NatU - Blank - Sample 1 ...**

1. Supported raw data file extension: **text (.TXT), ASCII (.ASC)**

**INSTRUCTIONS**

To run the processor simply execute function UThProcessor.m (no input arguments required). The following input window will appear:

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1. Select the **sample type** (sediment or sea water)
   * *Sediment*: tailing correction of 230Th counts
   * *Sea Water*: no tailing correction
2. Specify the **raw data folder** including the raw count files of each sample, blank and NatU measurement run (make sure aforementioned conditions are met!).
3. Specify the **number of analysis blocks.** Each analysis block comprises a number of sample runs preceded and followed by a blank run, e.g. *blank - 3 samples – blank.* Enter the number of blocks in the respective field.
4. Specify the **number of samples per block**. If the number of samples is the same for each block, a single value can be entered. If the number of samples varies between blocks, enter a value for each block separated by comma, semicolon, or space (if samples were analysed in 8 blocks comprising variable numbers of samples, 8 values need to be entered). Example: If the first 7 blocks consist of 3 samples and the last block consists of 4 samples the input required is **3,3,3,3,3,3,3,4** (see right-hand screenshot).
5. Specify a unique character sequence found in the sample-IDs (example: *JW,* cf. example file list)
6. Specify a unique character sequence found in the blank-IDs (default: *Blank*)
7. Specify a unique character sequence found in the NatU-IDs (default: N*atU*)
8. Choose whether or not to perform ID & particle flux calculations
9. Proceed

Based on the input, the analysis sequence will be generated and displayed in a separate window asking for confirmation:

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Hit “OK” to proceed. If the sequence is not in correct order hit “Cancel” and make sure the sorting of files in the raw data folder is in correct order (cf. Initial Conditions).

If ID and particle flux calculations are to be performed a second input window will appear. Bear in mind that this function outputs only values and **no errors** of 230Th and 234U concentrations as well as vertical particle fluxes. The error propagation of these calculation steps will be implemented in future releases.

A close up of a device

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For each sample enter (from left to right, any unspecified value needs to be written as “*NaN*”):

* Sample information
* Initial sediment weight in grams
* Sample age in years
* Water depth in meters
* Th parameters
  + 229Th spike weight in grams
  + 232Th concentration in ppm (TM measurement results)
  + 229Th:230Th isotope ratio of the spike (RY, **default value** given)
  + 229Th:230Th isotope amount ratio of the sample (RX, **default value**: 0)
  + 229Th concentration of spike in pg/g (CY)
* U parameters
  + 236U spike weight in grams
  + 238U concentration in ppm (TM measurement results)
  + 236Uh:234U isotope ratio of the spike (RY, **default value** given)
  + 236Uh:234U isotope amount ratio of the sample (RX, **default value**: 0)
  + 236U concentration of spike in pg/g (CY, **default value** given)

Once all the parameters have been specified hit the arrow button to proceed. The results will be displayed in tabular form and also stored as excel files in the raw data folder (subfolder: 'output').

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Excel file output:

1. 'SampleRatios.xls': Th and U isotope ratios per sample

* Th229\_230 (229Th/230Th ratio, tailing/blank/mass bias corrected)
* sigma\_Th229\_230 (standard deviation, sigma)
* sigmaP\_Th229\_230 (percentage standard deviation)
* U236\_234 (236U/234U ratio, tailing/blank/mass bias corrected)
* sigma\_U236\_234 (standard deviation, sigma)
* sigmaP\_U236\_234 (percentage standard deviation)

If ID/particle flux claulations have been performed

* Th230Conc (230Th concentration, ppm)
* sigma\_Th230Conc (not available, standard deviation, sigma, ppm)
* sigmaP\_Th230Conc (not available, percentage standard deviation, %)
* U234Conc (234U concentration, ppm)
* sigma\_U234Conc (not available, standard deviation, sigma, ppm)
* sigmaP\_U234Conc (not available, percentage standard deviation, %)
* FV (preserved vertical particle flux, g/m2/yr)
* sigma\_FV (not available, standard deviation, sigma, g/m2/yr)
* sigmaP\_FV (not available, percentage standard deviation, %)

Note, that in most cases the tailing corrected 230Th concentration ratio, STD and percentage of the procedural blank will be zero, yielding infinite Th229/Th230 ratios and STDs (shown as NaN in Matlab output and as empty cells in Excel output files).

1. 'NatURatios.xls': NatU isotope ratios
   * U235\_234 (235U/234U ratio, tailing/blank/mass bias corrected)
   * sigma\_U235\_234 (standard deviation, sigma)
   * sigmaP\_U235\_234 (percentage standard deviation)