## **Materials and Logs**

- analytik\_brunnen\_7\_kd.pdf
- iron\_hydroxide\_precipitation\_brunnen\_07.xlsx
- iron\_hydroxide\_precipitation\_brunnen\_07\_f1.xlsx
- iron\_hydroxide\_precipitation\_brunnen\_07\_f2.xlsx
  - auswertung-vor-ort\_paramter.xlsx
    - IsotopeData
    - sheet1.xlsx

## Software

You can process the data with the program AquaChem. The software is contained in a

## zip file

. Unzip the file into a folder AquaChem. You can open a folder Lubeca and modify/delete/add the existing sample by overwriting them with your data. Once data have been entered you can make Piper diagrams, Schoeller diagrams and run statistics and geochemical programs (PhreeqC).

The data can be processed with Diagramme. The software has been written in french but it has an English interface. Once the programme interface has been set to English all commands are given in English language. After you open the program Diagramme, you choose 'Langue' (fr. Language) and select English (or German, if you prefer ...).

There is a sample file called Luebeck.dia. It is zipped, you need to unzip it. With Diagramme you can open this file and add the data. It contains three dummy analyses that you can overwrite. With the programme Diagramme you can run hydrochemical programs and analyses.

## Task Log:

20.07.2016: (Yichen Xu) - All data are typed into excel files. Ion balance is calculated.

20.07.2016: (C. Kuells) - Software and template for hydrochemical analysis added.

25.07.2016: (Yichen Xu) - A general introduction is added. The example of ion balance and activity of ions calculation is added.

03.08.2016: (Yichen Xu) - The section of ion balance and activity calculation is completed.

07.08.2016: (Yichen Xu) - The section of saturation indices and the section of visualization are completed.

17.08.2016: (Yichen Xu) - The section of redox potential and the section of carbon balance are completed.

23.08.2016: (Yichen Xu) - The section of modeling is completed. The original data are updated to the latest version.

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