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NobleControl and Noble LabData: a measurement control system and a sub-database system for the post-processing of noble gas measurements in water samples

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A flexible measurement control system was developed to control noble gas measurements on water samples. The steps involved are i) separating all dissolved gases from water; ii) separating the noble gases (He, Ne, Ar, Kr, Xe) from reactive gases (like N_2 , O_2 , CO_2 , $CH_4...$); iii) separating noble gases from each other using cryo techniques and iv) measuring each noble gas in a dedicated mass spectrometer. The control software handles 86 pneumatic valves, 18 vacuum gauges, three cryo controllers, two Peltier controllers and three quadrupole mass spectrometers. It also contains a script language allowing flexible control and programming of different measurement processes. Status of the measurement system is controllable on-line in real time. This software generates approximately 70-100 MB per run of 48h of – in principle human readable – ANSI text files.

Furthermore, a database system was developed for raw data storage and post-processing of the noble gas measurements. This database system reads the text files and dispatches the values to a relational database system (MS SQL Server) with a total of 18 tables. These raw data (Volts and Amperes of mass spectrometer signals, Torrs of the gauges) are then fitted against time, background corrected and related to each other to obtain representative signals per inlet and isotope signal ratios. Many of these signals per inlet are then combined in a single post-processing to derive several day long time series of background, efficiency and linearity of the system for each species in question. At the end of the whole post-processing 70-100MB raw data are reduced to 16 numbers per unknown sample: the concentrations of gases (N₂, He, Ne, Ar, Kr, Xe) in ccSTP/g and the selected isotope ratios (20 Ne/ 22 Ne, 36 Ar/ 40 Ar, 38 Ar/ 40 Ar, 82 Kr/ 84 Kr, 83 Kr/ 84 Kr, 86 Kr/ 84 Kr, 129 Xe/ 132 Xe, 131 Xe/ 132 Xe, 134 Xe/ 132 Xe, 136 Xe/ 132 Xe).

The noble gas sub-database system is part of the laboratory management system LabData that contains subdatabases for stable isotopes, grain size analysis, gas chromatography and numerical codes for data interpretation like lumped parameter models of age distributions or noble gas palaeotemperatures (Suckow, 2012; 2013a; b; c; Suckow and Dumke, 2001). Both NobleControl and LabData are public domain software under the GNU-GPL licence and available from the author. The poster will present the underlying ideas and principles of the software.

References

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