Recent advances in the on-site analysis and process-based interpretation of dissolved (noble) gases in water bodies

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The gas concentrations in water bodies are controlled by air/water exchange, sources/sinks in the water, and mixing of different fluids. Atmospheric gases originate from air/water partitioning at the water surface and (partial) dissolution of air bubbles entrained/entrapped in the water (excess air, EA). The EA dissolved-gas concentrations are commonly substantial in groundwaters. The noble gas concentrations in water allow EA quantification, which provides a robust basis for quantitative interpretation of reactive gases.

We developed a membrane-inlet mass spectrometer [1] for quasi-continuous on-site gas analysis in the field (He, Ar, Kr, N_2, O_2, CO_2, CH_4, etc). Most recently, we miniaturized this instrument and reduced power consumption to allow battery operation in the field. This instrument yields gas concentration time series, which provide the data basis for robust interpretation and quantification of gas dynamics in terms of physical and biogeochemical processes (e.g., respiration/O_2 or denitrification/N_2).

Currently available software tools for physical interpretation of noble gas data are, however, not adequate to interpret data sets containing both noble and (bio)chemically active gases. The available tools are furthermore restricted to a limited and hard-wired set of physical gas-exchange processes. We therefore developed a new and flexible tool [2] (NOBLEFIT) for quantitative interpretation of dissolved gas data in terms of system-specific environmental processes and variables. NOBLEFIT covers the functionality of previous tools, but is designed to allow user-defined process models (e.g., physical conditions during atmosphere/water exchange, bubble/water interaction, strength and kinetics of internal gas sources and sinks, etc.).

Both on-site gas analysis and system-specific model fitting reflect significant improvements relative to currently available techniques. Moreover, the combination of both tools offers new avenues to study the interaction of physical and biogeochemical processes in water bodies and other environmental systems.

[1] Mächler et al 2012, *ES&T*, **10**.1021/es3004409 [2] Free software, http://sourceforge.net/projects/noblefit