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Impact of the volume of gaseous phase in closed reactors on ANC results and modelling

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The understanding of the geochemical behavior of polluted solid materials is often challenging and requires huge expenses of time and money. Nevertheless, given the increasing amounts of polluted solid materials and related risks for the environment, it is more and more crucial to understand the leaching of majors and trace metals elements from these matrices. In the designs of methods to quantify pollutant solubilization, the combination of experimental procedures with modeling approaches has recently gained attention. Among usual methods, some rely on the association of ANC and geochemical modeling. ANC experiments - Acid Neutralization Capacity - consists in adding known quantities of acid or base to a mixture of water and contaminated solid materials at a given liquid / solid ratio in closed reactors. Reactors are agitated for 48h and then pH, conductivity, redox potential, carbon, majors and heavy metal solubilized are quantified. However, in most cases, the amounts of matrix and water do not reach the total volume of reactors, leaving some space for air (gaseous phase). Despite this fact, no clear indication is given in standard procedures about the effect of this gaseous phase. Even worse, the gaseous phase is never accounted for when exploiting or modeling ANC data. The gaseous phase may exchange CO_2 with the solution, which may, in turn, impact both pH and element release. This study lies within the most general framework for the use of geochemical modeling for the prediction of ANC results for the case of pure phases to real phase assemblages. In this study, we focus on the effect of the gaseous phase on ANC experiments on different mineral phases through geochemical modeling. To do so, we use PHREEQC code to model the evolution of pH and element release (including majors and heavy metals) when several matrices are put in contact with acid or base. We model the following scenarios for the gaseous phase: no gas, contact with the atmosphere (open system) and real reactors conditions (semi-closed systems). The solid phases tested are pure phases (calcite, sulfides, etc.) and synthetic assemblages mimicking complex polluted matrices. The modeling clearly shows that the systems are sensitive to the opening to the atmosphere. If the open system and the system with no gas are entirely different, "real" reactors also differ significantly from the other systems. Apparently, the presence of the gaseous phase in reactors greatly impacts pH and element release. This parameter should be accounted for in ANC experimental procedures and modeling. In addition to this numerical study, experimental results, previously obtained for urban polluted sediments, are analyzed in lights of the findings of the numerical study. This step allows us to strengthen conclusions and to pinpoint at the necessity to account for the gaseous phase when performing and modeling ANC experiments.