Sulfur oxidation states in underground salt caverns and sedimentary formations: Geochemical considerations for underground H₂ storage

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Vast quantities of H₂ gas will be produced, stored, and retrieved in the zero-carbon global energy future. Underground salt caverns and porous sedimentary formations are storage options for H₂. A major concern inhibiting advancement of underground H₂ storage is the possibility of bacterial sulfate reduction, utilizing H₂ as the electron donor and generating H₂S gas, which is highly toxic and dangerous. In this work, the oxidation states of sulfur in salt dome samples and sedimentary formation samples were examined to increase understanding of the conditions for H₂S gas generation. Predominantly, mineral sulfur occurs in the +VI oxidation state, such as in gypsum, or the -I reduced state, such as in pyrite. Only oxidized sulfur can be used as an electron acceptor. We hypothesize that the sulfur minerals in the two types of geological formations are very different in oxidation state and are categorically different in terms of H₂S risk. We used the tender x-ray beamline (TES 8BM) at the NSLS-II synchrotron for x-ray absorption spectroscopy (XAS) and x-ray absorption near edge structure (XANES). This research is the first comparative analysis of sulfur oxidation in salt vs sedimentary rocks. We found that the salt formation rock samples uniformly contained sulfate minerals, and we conclude that safe and reliable storage of H₂ in salt caverns may be jeopardized if the risks are not thoroughly characterized. In contrast, we found that the sedimentary formation rock samples contained mostly disulfide minerals, and some evaporites and shales contained a mix of sulfur oxidation states. If H₂ is stored in these formations, the risk of H₂S gas is likely to be lower.