Effect of ionic strength on the kinetics of pyrite oxidation

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Pyrite (FeS_2) oxidation has been extensively studied for its role in the production of acid mine drainage [1-5]. Despite of all efforts important features of the oxidation reactions of FeS_2 are poorly understood. The present study investigates the effect of ionic strength on FeS_2 oxidation with dissolved oxygen.

Experiments were performed at 25 °C, $5.30 \leq$ initial pH ≤ 5.65 and 530 mV $\leq$ initial Eh $\leq$ 643 mV. NaCl was used to adjust the ionic strength (0-0.1 mol L^{-1}). Continuous agitation was performed during the reaction. The values of total dissolved sulfur concentration, electrical conductivity, Eh and pH of experimental solutions were periodically measured during mineral oxidation that lasted 100 hours. Dissolved iron concentrations could not be determined due to their extremely low values. Hence, the concentration of total dissolved sulfur was chosen as reaction progress variable.

It was found that the rate constant recorded between 10 hours and 100 hours is virtually independent of ionic strength. The average rate constant was determined to be 21.2±1.6 μmol m^{-2} h^{-1}.

The Fourier transform infrared spectroscopy data collected for reacted FeS_2 samples clearly indicate the formation of ferric oxyhydroxides on oxidized surfaces.

As expected, the rates of FeS_2 oxidation is not affected by ionic strength as long as the oxidant (O_2) has no charge [6]. Disulfide groups are oxidized with the production of unstable (thiosulfate and sulfite) and stable (sulfate) sulfoxyanions (see also [5]). Ferrous iron is easily oxidized by dissolved oxygen and transforms into ferric oxyhydroxides at pH≥4 [7-9].

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First-principles modelling of proton and proton coupled water transport in polymer electrolyte membranes

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In this presentation, results of research conducted in our group toward understanding various transport phenomena in polymer electrolyte membranes (PEMs) are presented. Polymer electrolyte membrane fuel cells (PEFC) have attracted interest due to its potential application for automobile and PEMs are a component for PEFC. Because the amount of electrical power generated by fuel cells is limited by the transport of protons, proton conduction in PEMs is a fundamental element that determines the performance of fuel cells. To understand proton transport and other related transport phenomena in PEMs, we have carried out a series of first-principle molecular dynamics simulations for Nafion and sulfonated polyether sulfones (SEPS), a hydrocarbon membrane.

Our simulations show that proton hopping probability does not depend much on the water content inside PEMs. This finding indicates that the classical *vehicular* diffusion model, which has been employed to account for the slow diffusion process of protons in the low water content Nafion, is an oversimplification. Furthermore, we found that difference in the value of proton diffusion coefficient with respect to water content inside PEMs is related to the different character of proton hopping occurring in water hydrogen bond network. Moreover, the results of the first-principles simulations allow us to explain the relationship between the proton dynamics and electro-osmosis (co-transport of water as a result of proton conduction) at an atomist level. Also, we compared transport properties of Nafion and SPES and found that at low hydration condition, SPES is not effectively hydrated by water molecules which hinders effective proton transport.

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