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Experimental process parameterization of a 3D site-scale model on effects of a compressed air intrusion into a shallow aquifer

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Abstract

Gases stored in the subsurface for balancing power fluctuations potentially escape from their reservoirs and affect protected groundwater resources. Here we presented an integrated experimental and modeling approach examining the site-scale effects of a compressed air leakage into a shallow aquifer. A main consequence may be pyrite oxidation, which can be strongly inhibited by surface passivation in carbonate-buffered aquifers. Based on laboratory results, predictions for changes in groundwater composition at site-scale and suggestions for a leakage monitoring were presented. Our study found this workflow consisting of experiments and numerical simulations to be valuable for predicting geochemical consequences of gas leakages.

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Keywords: pyrite oxidation; passivation; hydrogeochemical experiments; process simulation; site-scale modeling; compressed air energy storage; gas leakage; ANGUS+

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1. Introduction

The global transition towards sustainable energy sources, supported by ambitious national and international policies, predicts a continued increase in renewable power production. A major issue caused by the increasing share of renewable sources, such as wind turbines and solar panels, is the fluctuating electricity output of these technologies. The unstable gap developing between the current supply and the current demand in power networks may be balanced by various energy storage technologies integrated into energy networks. As a renewable share of 60-80% is scheduled to be reached to fulfill national, for instance German, greenhouse gas emission goals until 2050 [1], the magnitude of fluctuating gaps between power supply and demand is expected to increase. In case of the German example, when the national energy supply network will contain a renewable share of ca. 80%, a synergetic energy storage system is suggested to be a prerequisite for a technically stable and economically profitable power network operation [2].

In this storage concept, the development of geological energy storage technologies is foreseeable, and this development implies the construction of new, large-scale geological gas storage facilities in the upcoming decades [3,4]. The wide range of geological energy storage technologies includes storing heat or gases, each inducing a number of processes in the subsurface space used [5]. One of the most important, already operating, technologies is Compressed Air Energy Storage (CAES), where the surplus energy is conserved by compressing air and storing it in subsurface caverns or reservoirs [6,7].

Subsurface installations containing a stored gas under high pressure (e.g. wells, gas caverns, reservoirs, etc.) potentially cause accidental gas leakage events [8,9], which are amongst the unwanted side effects of gas storage operations. The geochemical effects of a gas intrusion into a shallow aquifer may lead to changes relevant for the operators of the gas storage site as well as for civil and official stakeholders [4,10]. An improved knowledge about geochemical processes, especially redox reactions, contributes to a better understanding of various aspects of routine operation and leakage management. The consecutive steps towards the characterization of reactions potentially following a leakage event may be realized through the collection and synthesis of literature and field data, laboratory experiments, process model development, and completed by numerical site-scale modeling, and pilot field investigations [11].

Leakage of compressed air may result in a high partial pressure of oxygen in aquifers that are typically depleted in oxygen. A major part of the oxygen intruding such an aquifer is usually consumed by the oxidation of pyrite [12], if reactive pyrite is available in sufficient amounts; therefore, pyrite oxidation can be considered as a potential main consequence of an accidental compressed air intrusion into a shallow aquifer. The knowledge on the kinetics of pyrite oxidation mostly originated from studies investigating acid mine drainage sites [13,14], where air-saturated meteoric water intrudes pyrite-rich geological units or mining waste deposits. The water percolating such reactive environments usually contains comparatively low concentrations of dissolved oxygen, such as in equilibrium with a gas phase having up to 0.21 bars of oxygen partial pressure. In contrast, in a scenario when compressed air stored underground leaks into a shallow aquifer, the groundwater may reach equilibrium with up to 10 bars of oxygen partial pressure, considering a total gas pressure of 50 bars at a depth of 500 m and the typical share of oxygen in the air gas mixture of approx. 21 %. The waters discharged from acid mine drainage environments are typically characterized by a low pH value and a high sulfate content, both resulting from pyrite oxidation. Williamson and Rimstidt [14] characterized the reaction rate of pyrite oxidation as proportional to the dissolved concentration of oxygen; therefore, a higher partial pressure of oxygen following a compressed air leakage may hypothetically result in higher pyrite oxidation rates and, therefore, even more significant changes in the composition of the groundwater compared to an acid mine drainage site. However, in shallow groundwaters the changes in pH may be buffered by dissolved - or even solid phase - carbonates nearly ubiquitously available in aquifers, which are typically not present in e.g. mining waste deposits [15]. Investigating the effects of such a pH buffer on pyrite oxidation kinetics is, therefore, essential for understanding the hydrogeochemical processes taking place after a compressed air leakage into a shallow aquifer.

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