The Coupled Simulation of CO_2 Fluid Flow and Chemical Reaction Focusing on Fe-Bearing Minerals

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A technology development of a fossil fuel power generation has made remarkable progress towards the reduction of CO_2 emissions. Above all, the so-called Oxyfuel combustion method of burning coal with Oxygen has attracted attention, because it can capture high-purity CO_2 containing almost no NOx (e.g. Uchida, 2014). In the Callide Oxfuel project conducted by Australian and Japanese public-private joint, the carbon capture technology was confirmed to be applied to a coal-fired power station to generate electricity with almost no emissions. Furthermore, the captured CO_2 was transported to the Otway research facility center operated by the CO2CRC in Victoria state located 2,200km away from Callide power station. Then CO_2 was injected into the saline reservoir in the demonstration test, which was the first demonstration test really seen in the world (Paterson, L.et al., 2013). The main purpose of this injection test was to reveal residual gas trapping mechanism using Pulsed Neutron Logging (PNL) and to study the impact on groundwater property due to injection of CO_2 captured by the Oxyfuel combustion method (Ennis-king et al., 2017; Haese et al., 2014). In the demonstration project, significant outcomes were obtained, such as a low impact on groundwater quality and a mechanism of chemical reaction between oxygen in the captured CO_2 and Fe-bearing minerals in the stratum (e.g. Todaka and Xu, 2017; Vu et al., 2018).

The geological candidate of CO_2 storage in Japan will be sandstone or tuff breccia. It is known that chlorite is one of the common minerals in sedimentary rocks and volcanic rocks in Japan, and its chemical properties vary site by site depending on the geological environment of the stratum (e.g. Kobayashi and Namanuma, 1960; Shiramizu, 1962). Especially, Japan is located in the complicated tectonic setting with various geological environments. Based on these findings, the authors consider that it is very important to take into account effects of not only siderite, pyrite and hematite but also chlorite which is a solid solution of clinochlore($Mg_5Al_2Si_4O_{10}(OH)_8$) and daphnite($Fe_5Al_2Si_4O_{10}(OH)_8$), when considering the chemical reaction between dissolved CO_2 with impurity of O_2 in groundwater and reservoir rocks As mentioned earlier, however, it is difficult to determine the chemical properties of chlorite in the formation. While employing numerical geochemical calculation is desirable in order to estimate the impact, the thermodynamic data of chlorite with Fe/(Mg+Fe) = 0.5, is only obtained by Xu et al. (2000). Then, in this research, the authors newly calculated the thermodynamic data of chlorite with various Fe/(Mg+Fe) ratios and reconsidered the results of the demonstration test in the Otway research facility center using published data. In this study, the simulator was employed TOUGHREACT V3-OMP developed by Lawrence Berkeley National Laboratory, United States. In addition, in order to focus on the phenomenon of the chemical reaction between dissolved CO_2 with impurity of O_2 in groundwater and reservoir rocks, we reproduced the state of the CO_2 plume in the reservoir using not only the pressure history matching but also result of PNL. Furthermore, in order to fully reflect groundwater properties in the reservoir to the numerical simulation, we employed the behavers of SO_4^{2-} as matching parameters, which affects the groundwater quality and SiO_2, and which is the main constituent of the stratum of pre-injected CO_2.

In this study, the solid solution of clinochlore and daphnite was considered, as a result, it was confirmed that the behavers of SO_4^{2-} and Fe^{2+} with the injecting CO_2 denote the same tendency of the case considering only clinochlore. As Todaka and Xu (2017) and Vu et al.(2018) mention, the result was also

shown that the chemical reaction related Fe was largely affected by the dissolution of pyrite and precipitation of hematite and goethite with O_2 as impurity. At the same time, these findings suggest that the impact for stratum in japan with injecting impurity CO_2 would be small.

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