A Brief Discussion on the Simulation of Thermal Storage Environment

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Abstract. The simulation process of thermal storage environment is divided into three parts: basic environment simulation of thermal storage, simulation of dissolution and precipitation of thermal storage minerals and experimental simulation of mixing of reinjection tail water and raw water. This paper introduces the simulation of temperature, pH, fluid mixing amount and reflection path in the basic environment simulation of thermal storage; the influence of temperature, pH and redox potential on the dissolution and precipitation law of mineral in thermal storage is mainly introduced.

1. Introduction

As a kind of resources, geothermal resources [1, 2] have the advantages of green, environmental protection, low-carbon and many advantages compared with the traditional resources. According to their types, they are mainly divided into shallow geothermal resources, hydrothermal geothermal resources and dry heat rock resources and so on. The unique medical care and recreational functions of geothermal water can attract tourists to come for sightseeing, recuperation, vacation, develop tourism, and diversify the local economic structure. However, due to its unreasonable exploitation and utilization and the difficulty of recharging, the amount of resources has decreased sharply. Therefore, how to reasonably and sustainably use underground hot water resources [3, 4] has become the research focus at this stage. Recharge [5-8] as the most direct and effective method has been highly valued by experts at home and abroad, and related simulation research is also carried out in an orderly manner. The simulation of the thermal storage environment is crucial to the study of recharge and its subsequent effects. Important, it not only affects the recharge volume, but also affects the properties of the target aquifer.

2. Simulation of the Basic Thermal Storage Environment

Due to the large burial depth, high water temperature and large changes of underground hot water, the density and pressure of the water change significantly. The groundwater continuously undergoes physical and chemical reactions with surrounding rocks during the migration process. Coupled with the influence of hot water extraction and cold water recharge, the dynamic field and temperature field of deep
underground hot water are complicated. Therefore, the rational development and utilization of geothermal resources requires a reasonable assessment of the amount of thermal storage resources, and the basis of the assessment is to simulate the basic environment of the thermal storage. It mainly includes the simulation of the four elements of thermal storage temperature, thermal storage pH, mixing amount of thermal storage fluid, and hydrogeochemical reaction path.

2.1. Thermal storage temperature simulation
The exploitation of underground hot water is a process of depressurization, cooling and degassing. Therefore, in the process of research and development and utilization of underground hot water, the temperature of deep thermal reservoirs must be reasonably estimated. Generally, the wellhead water temperature is lower than that of the thermal reservoir. In order to reasonably estimate the temperature of the thermal reservoir, the commonly used methods include direct measurement, geochemical temperature scale method, Na-K-Mg triangle diagram method, and multi-mineral equilibrium diagram method.

In the underground hot water system, the equilibrium constant of the reaction is affected by temperature, and the reaction temperature can be estimated from the equilibrium temperature. The geochemical temperature scale method estimates the thermal storage temperature based on the fact that the geothermal water reaches a chemical equilibrium with the minerals in the thermal storage under a specific temperature condition. Commonly used geochemical temperature scales [9] include Na-K temperature scale, K-Mg temperature scale and quartz temperature scale, among which Na-K temperature scale and K-Mg temperature scale are greatly affected by water-rock reaction conditions. Through the comparison of the simulated temperature and the measured temperature and the analysis of the related change trends, the appropriate thermal storage temperature scale method is selected.

The Na-K-Mg triangle diagram method can judge whether the hot water minerals are in equilibrium, and predict the thermal storage temperature when the water and rock reach equilibrium. This method is suitable for undisturbed or undisturbed deep underground hot water thermal storage temperature simulation.

The multi-mineral equilibrium diagram method is used to judge the overall chemical equilibrium state between underground hot water and rock minerals. The principle is to use the dissolved precipitation state of various thermal storage minerals in underground hot water, that is, the saturation index as a function of temperature. If these minerals are close to equilibrium at a certain temperature at the same time, it can be considered that these minerals have reached equilibrium with the underground hot water. The temperature at this time is the thermal storage temperature. The saturation index of thermal storage minerals at different temperatures can be simulated and calculated by PHREEQC software.

2.2. Thermal storage acid alkalinity simulation
Generally, the extraction of underground hot water is accompanied by the escape of CO₂ in the hot water, and the pH changes accordingly, resulting in a higher pH value of geothermal water at the wellhead than that of the hot water in the thermal reservoir. The actual pH value of underground hot water can be restored by using the PHREEQC software and the multi-mineral equilibrium diagram method.

2.3. Thermal storage fluid mixing simulation
Due to construction technology and technical limitations, during the underground hot water extraction process, low temperature water from other aquifers will be mixed to varying degrees, resulting in a difference between the wellhead water temperature and the actual thermal reservoir. Therefore, when reducing the heat storage temperature, the lower wellhead temperature caused by this part of the low temperature water should be considered.

2.4. Hydrogeochemical reaction path simulation
The reaction path simulation is mainly used to reflect the hydrogeochemical evolution of groundwater when the tail water of the mining well is recharged into the recharge well. According to the principle of conservation of mass, the chemical reaction that occurs in the process of flowing through is analyzed by
analyzing the change of water quality between the mining well and the reinjection well. It mainly includes two parts, one is the water chemistry evolution characteristics on the water flow reaction path, and the other is the identification of reactive minerals. The former mainly conducts comparative analysis of Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, SO₄²⁻, HCO₃⁻, TDS, etc. Reactive minerals are mainly determined based on the chemical composition of thermal storage minerals, thermal storage conditions and thermal storage lithology.

3. Thermal Storage Mineral Dissolution and Precipitation Simulation

The law of mineral dissolution and precipitation is usually studied and judged based on the mineral saturation index SI. When SI=0, the aqueous solution and the mineral are in equilibrium; when SI>0, the mineral is in supersaturation with respect to the aqueous solution; when SI<0, the mineral does not reach the saturated state with respect to the aqueous solution.

Using the water chemical composition detection data of the recharge well and the mining well, the saturation index of each mineral is calculated through the PHREEQC software. Thermal reservoirs usually contain plagioclase, muscovite, goethite, epidote, calcite, chaledony, kaolinite, dolomite, aragonite, quartz, orthoclase, barite, celestite, Strontium, anorthite, salt rock, illite, magnetite and montmorillonite-calcium, etc. According to different mineral properties and chemical composition, different types of minerals are selected as reactive minerals. There are many factors that affect the dissolution and precipitation of thermal storage minerals. The main factors are temperature, pH and redox potential.

4. The influence of temperature, pH value and redox potential on the law of mineral dissolution and precipitation

In the range of 0-200℃, the saturation index of carbonate minerals has a downward trend as the temperature rises. Calcite shows an upward trend when the temperature is higher than 90℃, but the saturation index of calcite, dolomite and strontium ore is always greater than zero. The saturation index of sulfate mineral gypsum does not change significantly with the increase of temperature; the saturation index of silicate minerals shows a downward trend as a whole, among which epidote has a tendency to precipitate with the increase of temperature and at lower temperatures. Although the saturation index of plagioclase is negatively correlated with temperature, there is always a tendency of precipitation. The saturation index of other minerals decreases with the increase of temperature; the saturation index of iron minerals has a downward trend as the temperature increases, but the saturation index of goethite is always greater than 0, which may be the main component of suspended solids in hot water.

The study of the deep geothermal water thermal storage environment in Xianyang City found that when pH>7, carbonate minerals begin to precipitate; the saturation index of sulfate minerals basically does not change with the change of pH, and the saturation index is always less than 0; However, most aluminosilicate minerals have a maximum saturation index SI at pH 6; goethite has a tendency to precipitate when the pH is greater than 3, while magnetite begins to precipitate when the pH is close to 10.

Among carbonate minerals, sulfate minerals, aluminosilicate minerals and iron minerals, the oxidation-reduction potential mainly has a greater influence on the saturation index of iron minerals, while it has less influence on the other three minerals.

5. Conclusions

The basic environmental simulation of thermal storage can determine thermal storage temperature, thermal storage pH, mixing amount of thermal storage fluid, and hydrogeochemical reaction path, which provides more realistic basic data for subsequent in-depth research. The simulation of the dissolution and precipitation law of thermal storage minerals can provide a basic basis for the hydrochemical characteristics and evolution of the groundwater in the study area [10], and it is also of general significance for studying how to improve the efficiency of geothermal tail water recharge.
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