Modeling of groundwater processes in a karstic aquifer of Sierra Madre Oriental, Mexico

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ABSTRACT

The Sierra Madre Oriental (SMO) is composed of ranges with important regional geological structures in highly fractured carbonate rocks (Abra Formation), which facilitate the recharge of aquifers. At the regional scale, recharge occurs in the western SMO and locally, in ranges such as Palmillas, La Colmena and Abra, while the regional discharge is to the east in the Huasteca zone. Intermountain valleys, such as El Salto, are located near the regional discharge zone. Three end members were identified in these regions, one related to local flow, another to intermediate and a third to regional flow. These flows define ternary mixing processes in groundwater. In this paper, the evolution of groundwater is studied, which is important for learning the system performance and hydrogeochemical processes through VISHMOD (Virtual Samples in Hydrochemical Modeling) methodology. The mixing model for the intermountain valleys indicates that many recharges occur, for which local flow contributes 68.3%, intermediate flow 12.3% and regional flow 19.4%. The inverse modeling shows that the water-rock interaction, precipitation and/or dissolution of calcite, gypsum and dolomite are the main processes occurring in the aquifer system of the intermountain valleys.

1. Introduction

The chemical composition of groundwater is mainly controlled by factors such as residence time, distance, mixture, mineralogy and geology of the aquifer. The evolution of groundwater begins when rainwater seeps into the land and is enriched with ions due to interaction with the geological environment during its path. This interaction produces different chemical compositions in the groundwater, based on which different types of groundwater families can be identified. Evolution of groundwater can be studied using tools such as hydrogeochemistry, particularly conservative elements, which are considered tracers. This evolution can be handled as mixing end members, where the starting point is the recharge and discharge is the end (Morán-Ramírez et al., 2013, 2016; Moran-Ramirez and Ramos-Leal, 2014; Ledesma-Ruiz et al., 2015). In numerous publications, the amount of mixing between freshwater and seawater or between groundwater from different sources has been evaluated (Dixon and Chiswell, 1992;

Genereux et al., 1996; Laaksoharju et al., 1999; Lee and Krothe, 2001; Ramos-Leal et al., 2007; Gómez et al., 2008; Petitta et al., 2010; Hernández-Antonio et al., 2015). These mixing models are identified by end members (EM) containing the extreme (maximum and minimum) chemical concentrations in the hydrogeological system. This identification using EM is based on conservative elements that do not interact with the environment. To assess water rock interaction, the tool used is chemical modeling, in which physical and chemical principles are applied to the simulation of the system. The main objective of modeling is to create or devise theoretical reaction models that can provide elements to explain that which is observed in nature. These models are constructed using chemical composition in the aqueous phase, isotope geology and the mineralogy of the system (Lee and Krothe, 2001; Hidalgo and Cruz, 2001; Abu-Jaber, 2001; André et al., 2004; Hereford et al., 2007). Chemical modeling can be performed in two ways: 1) direct modeling, which involves predicting the water composition and the mass transfer that could result from hypothetical reactions, and 2)

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inverse modeling, which applies to inverse modeling of field samples along a flow line. However, no work to date has used only hydrochemical modeling of EM. Nevertheless, in these studies, mixing processes do not explain the final composition of groundwater. In addition, few studies have included the application of direct modeling of water-rock interactions and inverse modeling to explain and understand the physicochemical processes occurring in groundwater (Helgeson et al., 1970; Plummer and Back, 1980; Plummer et al., 1988; Parkhurst and Apello, 1999; Hidalgo and Cruz, 2001; André et al., 2004; Hereford et al., 2007).

In this paper, VISHMOD (Virtual Samples in Hydrochemical Modeling) methodology (Moran-Ramirez and Ramos-Leal, 2014) is used to understand the evolution of groundwater, which can be represented as a mixture of two or more EM, to identify water-rock interaction processes that occur in the system which give rise to the chemical signature of water at each site. The so-called VISHMOD methodology, which unlike other models uses virtual samples constructed from the sum of the mixing fractions of each EM (Moran-Ramirez and Ramos-Leal, 2014).

In general, VISHMOD methodology models are based on mixtures with a small number of representative samples (EM) of the overall system that represent the behavior of groundwater during its evolution. In this methodology, the processes occurring in the hydrogeochemical evolution, such as mixing, water-rock interaction are identified.

In some cases, it is not possible to apply inverse modeling in the first instance, so VISHMOD methodology is useful to identify the processes that occur before applying the inverse modeling. The hydrogeochemical models in hydrogeological systems need to be calibrated. The VISHMOD methodology makes standardization and control possible to demonstrate the degree to which a model is able to reproduce field measurements (Moran-Ramirez and Ramos-Leal, 2014).

The study area is located in San Luis Potosi State, Mexico, in the area known as Huasteca. Located in the central part of the Sierra Madre Oriental (SMO), bordering the Gulf of Mexico, this area is mainly composed of limestone karst, with north-south folds forming intermountain valleys (Fig. 1). This region is considered to be part of the discharge area of the SMO (Moran-Ramirez et al., 2012, 2013). In general, the knowledge on the hydrodynamics of karstic system is poor because this area is difficult to study due to steep terrain, excessive vegetation and the absence of extraction wells. The availability of groundwater in the area depends on climatic conditions and the topography of the intermountain region, as well as the physical characteristics of the subsurface. In this work, inverse modeling is performed between a virtual sample (Composition 1) obtained from the EM and the actual sample (Composition 2).

With this methodology, work arises from a mixing model for possible hydrogeochemical processes (dissolution and precipitation of minerals, ion exchange, terms of acidity and basicity, redox, etc.) leading to the chemical composition of the system. The main objective of modeling is to create or devise theoretical reaction models that can provide elements to explain that which is observed in the actual system.

2. Methodology

2.1. Field and laboratory work

Hydrogeochemical data were determined in March 2010 from samples of 27 wells, springs and hand dug wells in the southern study area, in the municipality of Naranjo (Fig. 1 and Table 1). The springs are located in the limestone of El Abra Formation, while the dug wells are in shales and the thinly layered argillaceous limestone of the San Felipe Formation. The wells are located in both formations.

Water samples to determine anions were collected in 60 ml polyethylene bottles (HDPE) and washed and rinsed 7 times with deionized water, whereas the bottles for samples used to determine cations were washed with 10% HCl and rinsed 7 times with deionized water. Water samples to determine cations and Sr were acidified with concentrated HNO_3 (pH < 2), whereas the samples to determine anions were not acidified. All samples were preserved at a temperature below 4 °C until laboratory analysis. Field measurements included pH, electrical conductivity, alkalinity by titration, redox potential (RP), dissolved oxygen (DO), total dissolved solids (TDS) and temperature (T).

The chemical composition of the water samples was determined at the Geoscience Laboratory Center, National Autonomous University of Mexico. Cations (Ca^{2+}, Mg^{2+}, Na^+ and K^+) and Sr were determined by Inductively Coupled Plasma-Atomic Emission Spectroscopy (Model Thermo ICP-AES 6500Duo) and anions (Cl^- and SO_4^{2-}) were determined by colorimetric at the Institute for Scientific and Technological
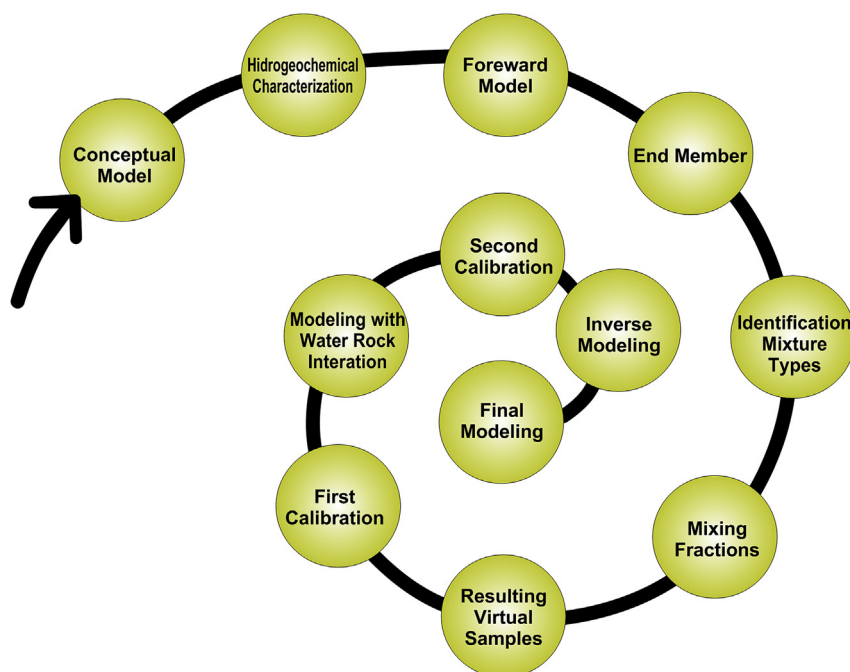

Fig. 1. Flowchart of modeling strategy of VISHMOD methodology.