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3D mapping, hydrodynamics and modelling of the freshwater-brine mixing zone in salt flats similar to the Salar de Atacama (Chile)

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ABSTRACT

Salt flat brines are a major source of minerals and especially lithium. Moreover, valuable wetlands with delicate ecologies are also commonly present at the margins of salt flats. Therefore, the efficient and sustainable exploitation of the brines they contain requires detailed knowledge about the hydrogeology of the system. A critical issue is the freshwater-brine mixing zone, which develops as a result of the mass balance between the recharged freshwater and the evaporating brine.

The complex processes occurring in salt flats require a three-dimensional (3D) approach to assess the mixing zone geometry. In this study, a 3D map of the mixing zone in a salt flat is presented, using the Salar de Atacama as an example. This mapping procedure is proposed as the basis of computationally efficient three-dimensional numerical models, provided that the hydraulic heads of freshwater and mixed waters are corrected based on their density variations to convert them into brine heads. After this correction, the locations of lagoons and wetlands that are characteristic of the marginal zones of the salt flats coincide with the regional minimum water (brine) heads.

The different morphologies of the mixing zone resulting from this 3D mapping have been interpreted using a two-dimensional (2D) flow and transport numerical model of an idealized cross-section of the mixing zone. The result of the model shows a slope of the mixing zone that is similar to that obtained by 3D mapping and lower than in previous models. To explain this geometry, the 2D model was used to evaluate the effects of heterogeneity in the mixing zone geometry. The higher the permeability of the upper aquifer is, the lower the slope and the shallower the mixing zone become. This occurs because most of the freshwater lateral recharge flows through the upper aquifer due to its much higher transmissivity, thus reducing the freshwater head. The presence of a few meters of highly permeable materials in the upper part of these hydrogeological systems, such as alluvial fans or karstified evaporites that are frequently associated with the salt flats, is enough to greatly modify the geometry of the saline interface.

1. Introduction

Salt flats (*salares*) are an important source of minerals. They account for half of the world's lithium production and contain the main economic reserves of this element (USGS, 2017). In addition, boron and potash are economically mined from salt flats. Lithium is a strategic commodity; its uses vary from light batteries to cancer treatment. Its demand has notably increased in the last decade, and this trend will probably continue in the future (Vikström et al., 2013), as large quantities may be needed to develop nuclear fusion reactors using tritium generated from lithium. This fact is evidenced by the large number of countries that are just now commissioning studies to determine the mineral potential of their salt flats (e.g., Salar de Uyuni in Bolivia or Salar del Hombre Muerto in Argentina) as well as to increase the amounts of resources that could be exploited during current mining activities (e.g., Salar de Atacama in Chile). This explains the current worldwide interest in salt flat hydrogeology, which is also due to the existence of peripheral brine and saline water lagoons that have high ecological, human and tourist value, in addition to their scientific value.

Salt flats are endorheic lagoon systems associated with arid or hyperarid climates, where the rate of evaporation is very high; in many

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cases, this causes the surface water to disappear and the water table to lie just below the land surface (Yechieli and Wood, 2002). This characteristic is what triggers the important precipitation or accumulation of high-value industrial minerals (Corenthal et al., 2016; Kesler et al., 2012; Munk et al., 2016; Risacher et al., 2003). In these endorheic basins, it is common for evaporation to be higher than local recharge (Hardie, 1991); thus, some other contribution, which is often groundwater, may compensate for this difference. In the simplest case, ignoring hypothetical deep contributions or inflows from other basins, the only water input to the salt flat system is lateral inflow and direct rainfall (which is minor due to the aridity of the climate), and the only output from the system is evaporation. These factors are all strongly related to climate variability and could potentially be affected by global climate change (Rosen, 1994).

The most accepted hydrogeological model assumes that dense brines produced from surface evaporation overturn and sink in the central area of the salt flat, setting up large-scale convection cells in its nucleus (i.e., the core of the salt flat, which is dominated by halite). These cells return to the surface at the margins of the salt flat, where the brines mix with incoming fresh groundwater in a complex process (Fan et al., 1997; Hamann et al., 2015; Nield et al., 2008; Wood and Sanford, 1990; Wooding et al., 1997). For this reason, the discharge of groundwater essentially occurs at the resulting freshwater-brine mixing zone areas, where lagoons may appear (Duffy and Al-Hassan, 1988; Tejeda et al., 2003). As a result, wetlands are commonly present in the margins of salt flats and are the bases for complex and sensitive ecological habitats surrounded by barren lands.

The contact between two miscible fluids of different densities is characterized by a mixing zone, which is also called a saline interface. This interface results from the dynamic equilibrium of moving fresh- and saltwater (Custodio and Bruggeman, 1987; Custodio and Llamas, 1976; Dentz et al., 2006), where the relationship between the concentrations of both fluids is stoichiometric.

In coastal aquifers, the position and characteristics of the mixing zone are well known, and its upper part coincides with the coastline in water table aquifers (Bear, 1972; Glover, 1959; Werner et al., 2013). In salt flats, where the density contrasts are much greater than those in coastal aquifers, the mixing zone develops as a result of point pressure equilibrium between recharge and evaporated water, but its position and geometry are more difficult to predict. This is because the brine in the salt flats is generated *in situ* as a result of evaporation (Acosta and Custodio, 2008), and recharge and evaporation are strongly subject to climatic oscillations (Tyler et al., 2006). Brine mining can affect the dynamics of the mixing zone in a short period of time, similar to freshwater extraction in coastal aquifers (Oude-Essink, 2001). In the natural state, evaporation occurs in both the salt flat nucleus and the marginal zone, regardless of whether it is a sheet of open water (marginal lagoons) or a shallow water table, which commonly have very irregular spatial distributions.

The need to assess the detailed characteristics of the mixing zone occurs immediately when managing both mineral resources and their associated ecosystems. The best management tool are the numerical models in which the effects of variable density are taken into account. These models are expensive to run in two-dimensional (2D) cases and are currently very difficult to run in three-dimensional (3D) cases at the regional scale (Oude-Essink and Boekelman, 1996). Nevertheless, 3D regional scale models are needed for the management of any hydrogeological system. In the case of coastal systems, this problem is solved in two ways: (1) neglecting the effects of variable density by assuming some simplifications or (2) converting the pressures of marine and variable-density waters into equivalent pressures of freshwater (Lu et al., 2015; Maas and Emke, 1989). The last solution, despite providing only an approximation of the actual situation (Post et al., 2007), is the one that has been chosen to model many coastal systems. However, to date, there is no evidence that any similar methodology has been proposed for the study and management of salt flats. Furthermore, the simplifications that are frequently assumed in coastal aquifers, such as neglecting density variations when advection is dominant over convection (Iribar et al., 1997; Vázquez-Suñé et al., 2006), are not acceptable in salt flats.

To obtain solutions for the above problem, the Salar de Atacama (NE Chile) was chosen as a case study. The choice was based on three characteristics: (1) it is the third largest salt lake on Earth, with a surface area of 3000 km^2; (2) it contains exceptional water ecosystems and bird nesting areas in the surficial mixing zone area, which require scientific solutions for their preservation and sustainability; and (3) there is a unique monitoring network that is regularly operated and well instrumented (Tyler et al., 2006) thanks to the exploitation of brine resources carried out in the southwestern area of the salt flat nucleus.

The main objective of this work is to obtain the first 3D map of the salt flat mixing zone, using the Salar de Atacama as a case study. This 3D map, together with an idealized 2D numerical model, allows us to understand the dynamics of the mixing zone and the effects of heterogeneity on its large-scale geometry. We also propose the use of the 3D map to apply simplified rules for constant-density 3D models that include mixing zones.

The structure of the manuscript follows the order described below. First, the 3D mapping of the mixing zone is addressed. Second, the usefulness of 3D mapping in the salt flats to correct the hydraulic heads by density differences and to facilitate their modelling at a constant density is shown. Third, the idealized 2D numerical model of the regional mixing zone is performed. Fourth, the sensitivity analysis of the hydraulic conductivity of the upper aquifer is carried out to determine its influence on the geometry of the mixing zone on a regional scale.

2. Materials and methods

2.1. Geographic setting

The Salar de Atacama (hereinafter SdA) is located in northern Chile between 23° and 24° South latitudes and 68° and 69° West longitudes; it is located in Region II (Antofagasta) and within the limits of the community (municipality) of San Pedro de Atacama (Fig. 1). The basin where the salt flat is located has an oval shape, with the long axis in the N-S direction and an extent of approximately 20,000 km^2. It is bordered to the west by the Cordillera de la Sal (Salt Range), which stretches from NNE to SSW at the slopes of the Domeyko Range, and to the East by the western Cordillera de los Andes (Andean Range), whose high peaks are crowned by the current volcanic arc (> 5500 m a.s.l., metres above sea level). The northern part of the basin is bounded by the merging of the Domeyko Range and the Andean Range, while the southern part is bounded by the Lila Mountains.

Because the Andean Range acts as a geographic barrier to atmospheric movement, the SdA is characterized by a hyperarid climate, resulting in a very low rainfall rate (Bookhagen and Strecker, 2008; Garreaud et al., 2010; Hartley and Chong, 2002). On average, the salt flat receives less than 20 mm/yr of precipitation. The major water source is groundwater coming from the Andean Range. In the mountains, the average precipitation reaches 160 mm/yr (IDAEA-CSIC, 2017). The output is water table evaporation produced in the nucleus and marginal zone, where the mean surficial water evaporation rate is 4.3 mm/d. Evaporation decreases as the depth of the water table increases, and it depends on the soil composition (Kampf et al., 2005; Kampf and Tyler, 2006; Muñoz-Pardo and Ortiz-Astete, 2004).

The two main river courses contributing to the salt flat, as shown in Fig. 1, are the San Pedro River, which has an average flow of 1 m^3/s and torrential events of up to 25 m^3/s, and the Vilama River, which has an average flow of 0.2 m^3/s. These rivers flow from North to South (Salas et al., 2010). The San Pedro River ends in a delta with the same name, while the Vilama River disappears in the upper half of its basin. There are also some intermittent streams that descend from the mountains and infiltrate into the extensive alluvial fans on the eastern side of the