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Maximizing the value of pressure data in saline aquifer characterization

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ABSTRACT

The injection and storage of freshwater in saline aquifers for the purpose of managed aquifer recharge is an important technology that can help ensure sustainable water resources. As a result of the density difference between the injected freshwater and ambient saline groundwater, the pressure field is coupled to the spatial salinity distribution, and therefore experiences transient changes. The effect of variable density can be quantified by the mixed convection ratio, which is a ratio between the strength of two convection processes: free convection due to the density differences and forced convection due to hydraulic gradients. We combine a density-dependent flow and transport simulator with an ensemble Kalman filter (EnKF) to analyze the effects of freshwater injection rates on the value-of-information of transient pressure data for saline aquifer characterization. The EnKF is applied to sequentially estimate heterogeneous aquifer permeability fields using real-time pressure data. The performance of the permeability estimation is analyzed in terms of the accuracy and the uncertainty of the estimated permeability fields as well as the predictability of breakthrough curve arrival times in a realistic push-pull setting. This study demonstrates that injecting fluids at a rate that balances the two characteristic convections can maximize the value of pressure data for saline aquifer characterization.

1. Introduction

Accurate estimates of hydrogeological parameters in subsurface flow and solute transport models are critical for making predictions and managing aquifer systems. The process of estimating model input parameters, such as permeability and porosity, from observational data is often referred to as an inverse problem. Over the past few decades, various inversion methods have been proposed for groundwater modeling, and current methods are advanced enough to handle stochastic, nonlinear, and large-dimensional problems (Carrera et al., 2005; Fienen et al., 2008; Hochstetler et al., 2016; McLaughlin and Townley, 1996; Oliver and Chen, 2011; Yeh, 1986; Zhou et al., 2014). The ensemble Kalman filter (EnKF) is one such method that has gained popularity for aquifer characterization because it is easy to implement and can efficiently incorporate real-time data from a monitoring system, allowing for dynamic data assimilation (Aanonsen et al., 2009; Zhou et al., 2014). The first application of the EnKF to subsurface modeling problems was in petroleum engineering (Geir et al., 2005; Gu and Oliver, 2005; Nævdal et al., 2002); it has since been successfully extended to groundwater applications (Chen and Zhang, 2006).

The first groundwater application of the EnKF was in using groundwater flow information, such as hydraulic head data, to estimate permeability fields (Chen and Zhang, 2006; Hendricks Franssen and Kinzelbach, 2008; Tong et al., 2010). However, in a constant density groundwater flow, pressure data alone are often not sufficient to accurately estimate permeability fields; accurate estimation requires time-dependent pumping tests (Cardiff et al., 2013; 2012; Li et al., 2005) or additional data sets, such as tracer transport data (Kang et al., 2016b; Lee and Kitanidis, 2014; Li et al., 2012a; Zhang et al., 2014). The EnKF has been successfully used to incorporate multiple data sets for permeability characterization in constant density groundwater flow (Li et al., 2012a; Liu et al., 2008; Schöniger et al., 2012; Xu and Gómez-Hernández, 2016; Xu et al., 2013; Zhou et al., 2011). However, there are few inverse modeling studies of heterogeneous permeability fields in a scenario with variable-density groundwater flow and solute transport; this scenario is important for coastal aquifers experiencing

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seawater intrusion and for managed aquifer recharge (MAR) applications in saline aquifers (Bastani et al., 2010; Kang et al., 2017b; Pool et al., 2015).

As seawater intrusion and freshwater shortages intensify, MAR is becoming an attractive technology for many coastal saline aquifers worldwide (Simmons, 2005). The coupling between fluid pressure and the spatial salinity distribution is significant in variable-density flow because the spatial salinity distribution determines the spatial fluid density distribution (Massmann et al., 2006; Simmons, 2005; Simmons et al., 2001; Ward et al., 2007; Werner et al., 2013; Zuurbier et al., 2014). This coupling between the salinity-controlled, density-driven flow and the salinity evolution leads to a time-dependent pressure; consequently, transient pressure data can be more informative for estimating aquifer permeability than in density-invariant cases (Carrera et al., 2010). Although many studies have shown the density effects on groundwater flow (Beinhorn et al., 2005; LeBlanc et al., 1991; Müller et al., 2010; Shakas et al., 2017; Vereecken et al., 2000), the variable-density effect on the value of pressure data has not been systematically studied. The first attempt to exploit this property for saline aquifer characterization was made by Kang et al. (2017b), who estimated the heterogeneous permeability field of a saline aquifer using fluid pressure data from an observational network consisting of multiple wells with pressure gauges at multiple depths. For a fixed freshwater injection rate, the authors showed that the quality of the inverse estimation does indeed improve as the density contrast between injected freshwater and the initial saline groundwater increases.

Ward et al. (2007) showed that the significance of variable-density effects during injection depends on the mixed convection ratio, which is a ratio between two characteristic types of convection: free convection due to density contrast, and forced convection due to a hydraulic gradient. For a given saline aquifer, typically there is little control over free convection because the site-specific ambient groundwater salinity determines the density contrast between injected freshwater and the ambient groundwater. However, forced convection can be controlled by human operations such as injection; thus the mixed convection ratio can be engineered by changing the freshwater injection rate.

The goal of this study is to systematically investigate how the freshwater injection rate impacts the usefulness of transient pressure data for saline aquifer characterization. To simulate a saline aquifer system where flow occurs due to the density difference between the ambient saline groundwater and injected freshwater, we developed a 2D density-dependent flow and transport model. An EnKF with covariance localization and inflation was then employed to sequentially estimate heterogeneous aquifer permeability fields using real-time pressure data. The performance of the permeability estimation was analyzed in terms of the accuracy and the uncertainty of the estimated permeability fields, and in terms of the ability of the model to predict breakthrough curve arrival times in a push-pull flow configuration not used during the estimation. The main contribution of this study is in elucidating the density effects on the value-of-information in pressure data over wide range of mixed convection regimes. To the best of knowledge, this is also the first study applying EnKF to a saline coastal aquifer system. Although this analysis was conducted for a coastal saline aquifer domain, the results are widely applicable to aquifer management and other subsurface applications in which density-driven flow is important, such as CO_2 storage and sequestration, seawater intrusion, and MAR in brackish/saline aquifers.

In Section 2 we describe the theoretical framework of mixed convection analysis for variable-density aquifer problems. In Section 3 we present the numerical model for simulating variable-density flow and transport, followed by a description of the ensemble-based data assimilation algorithm of the EnKF with covariance localization and inflation. In Section 4 we present three synthetic case studies with different types of permeability fields and monitoring networks under various mixed convection regimes. Finally, we summarize our conclusions and guidelines for future work in Section 5.

2. Mixed convection analysis

We examine a standard aquifer domain known as Henry's problem (Henry, 1964), which has been used to develop analytical and numerical approaches for considering variable-density effects (Abarca et al., 2007; Abd-Elhamid and Javadi, 2011; Frind, 1982; Huyakorn et al., 1987; Lee and Cheng, 1974; Pool and Carrera, 2011; Rastogi et al., 2004; Segol et al., 1975). Fig. 1 shows a schematic illustration of the aquifer domain and boundary conditions.

The aquifer is initially fully saturated with saline groundwater. Freshwater is injected from the domain's left boundary, while a hydrostatic pressure distribution is imposed on the right boundary. In the aquifer, fluid flow is initiated by the hydraulic gradient caused by the freshwater injection; this flow is the forced convection. For forced convection, a characteristic velocity can be defined as

$$v_{\text{forced}} = \frac{Q}{B\phi}, \tag{1}$$

where ϕ is the porosity, B is the aquifer depth in the z direction, and Q is the freshwater injection rate into a cross section of height B and unit thickness. The density difference between the injected freshwater and the ambient saline groundwater also contributes to the fluid flow; this flow is the free convection. For free convection, a characteristic velocity can also be defined as

$$v_{\text{free}} = \frac{k\Delta\rho g}{\mu\phi}, \tag{2}$$

where k is the mean permeability, $\Delta\rho$ is the density difference between the injected freshwater and initial groundwater, g is the gravitational constant, and μ is the dynamic viscosity of the fluid.

Ward et al. (2007) found that the importance of density effects depends on the interplay between forced and free convection. They introduced the mixed convection ratio, M, a dimensionless number defined as the ratio of the characteristic velocity of free convection due to density contrast to the characteristic velocity of forced convection due to freshwater injection:

$$M = \frac{v_{\text{free}}}{v_{\text{forced}}} = \frac{k\Delta\rho g B}{\mu Q}. \tag{3}$$

Mixed convective regimes can be characterized according to the mixed convection ratio. When $M \sim 1$, free and forced convection are balanced and the two characteristic velocities are approximately equal. Forced convection dominates the flow in the system when $M \ll 1$, and free convection dominates when $M \gg 1$. The tilt of the freshwater-saltwater interface increases with increases in the mixed convection ratio. Note that when there is no density difference between the injected and ambient fluids, $M = 0$.

For a given saline aquifer, we do not have control over free convection which is determined by the site-specific ambient groundwater salinity. Therefore, the freshwater injection rate determines how important the effects of density variations are, as represented by the mixed convection ratio. In order to systematically investigate how the freshwater injection rate impacts the usefulness of transient pressure data for heterogeneous permeability estimation, we use pressure data to estimate heterogeneous permeability fields in different mixed convective regimes. In the next section, we describe a forward numerical model for simulating variable-density flow and transport, and we develop a data assimilation model based on the EnKF to sequentially estimate heterogeneous permeability fields.