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Optimization of groundwater sampling approach under various hydrogeological conditions using a numerical simulation model

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ABSTRACT

This study presents a numerical model based on field data to simulate groundwater flow in both the aquifer and the well-bore for the low-flow sampling method and the well-volume sampling method. The numerical model was calibrated to match well with field drawdown, and calculated flow regime in the well was used to predict the variation of dissolved oxygen (DO) concentration during the purging period. The model was then used to analyze sampling representativeness and sampling time. Site characteristics, such as aquifer hydraulic conductivity, and sampling choices, such as purging rate and screen length, were found to be significant determinants of sampling representativeness and required sampling time. Results demonstrated that: (1) DO was the most useful water quality indicator in ensuring groundwater sampling representativeness in comparison with turbidity, pH, specific conductance, oxidation reduction potential (ORP) and temperature; (2) it is not necessary to maintain a drawdown of less than 0.1 m when conducting low flow purging. However, a high purging rate in a low permeability aquifer may result in a dramatic decrease in sampling representativeness after an initial peak; (3) the presence of a short screen length may result in greater drawdown and a longer sampling time for low-flow purging. Overall, the present study suggests that this new numerical model is suitable for describing groundwater flow during the sampling process, and can be used to optimize sampling strategies under various hydrogeological conditions.

1. Introduction

Groundwater resource is critical in sustaining the lives of billions of people, but it is being exploited at an unsustainable rate (Gleeson et al., 2012). Groundwater contamination due to industrial and agricultural activities is worsening the situation (Huang et al., 2017; Ma et al., 2016). Groundwater monitoring is important for determining the source and spatial extent of groundwater contamination (Cal-DTSC, 2008), the temporal trend (Grimmeisen et al., 2016), optimum remediation design (Hou and Leu, 2009; James and Gorelick, 1994), and monitored natural attenuation (Chiu et al., 2013). The burden associated with groundwater monitoring is high. A typical large contaminated site usually has hundreds of groundwater monitoring wells, and regular groundwater monitoring at a single site may cost up to $10 million per year (Johnson et al., 1996). Given that hundreds of thousands of contaminated sites exist globally (European Commission, 2014; USEPA, 2004), research and development pertaining to groundwater monitoring can render significant social and economic gains.

In the field of groundwater monitoring, industrial practitioners and regulators are facing two major challenges: (1) how to optimize the sampling method and monitoring strategy to reduce its cost; (2) how to ensure the monitoring results are representative of true condition in the formation thus allowing informed decision making. Over the past two decades, researchers have conducted extensive research aiming at optimizing groundwater monitoring network (Aziz et al., 2003), reducing sampling frequency (Barcelona et al., 1989; Johnson et al., 1996), developing and deploying more efficient sampling techniques like low-flow purging method (Puls and Barcelona, 1996) and passive samplers (Britt et al., 2010; ITRC, 2006; Powell and Puls, 1993), as well as better understanding contaminant migration during the sampling process (Barcelona et al., 2005). However, there are still many gaps between research and practice regarding groundwater monitoring, especially regarding groundwater sampling methods.

Two groundwater sampling methods are the most widely used nowadays: the low-flow method and the well-volume method (Cal-DTSC, 2008; USEPA, 2002). In the low-flow sampling method,

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water quality indicators (e.g., pH, temperature, turbidity, dissolved oxygen (DO), specific conductance, oxidation-reduction potential (ORP)) are measured in real-time as groundwater is being pumped out of a monitoring well, and if three successive readings are stable, then the water being purged is considered representative of aquifer water (Garske and Schock, 1986). This method is advantageous because it minimizes disturbance to well water, reduces the amount of hazardous wastewater generated, and often reduces time thus labor cost required to collect each sample. The low-flow method is often favored by practitioners and also recommended by regulators (USEPA, 2002). Even though the low-flow method was originally designed for sampling small vertical intervals (USEPA, 2002), researchers have suggested that it is suitable in many more situations (Barcelona et al., 2005). When the low-flow method is not suitable, professionals often choose to use the well-volume method, in which a pre-determined well volume (e.g. three bore volumes) of water is purged out prior to a representative groundwater sample being collected. This method is also technically rigorous but is often associated with high cost due to longer sampling time and a large volume of hazardous wastewater.

Low-flow groundwater sampling is challenging in that there are many "rules-of-thumb" in regulatory guidance that are either vague or solely based on qualitative and empirical evidence. For instance, the USEPA recommends that water level drawdown in low flow purge should be less than 0.1 m (USEPA, 2002). But this criterion is often not met in reality and the USEPA recognize that this criterion may be difficult to meet "due to geologic heterogeneities within the screened interval". Therefore, the USEPA recommends "adjustment based on site-specific conditions and personal experience". This poses a challenge to industrial practitioners who design and implement groundwater monitoring plans, as well as regulators who oversee and examine the quality of groundwater monitoring programs, because there is no well documented scientific evidence for professionals to make informed decision based on such "site-specific conditions and personal experience". Some researchers have developed models to simulate groundwater flow regime in sampling scenarios (Martin-Hayden, 2000b; McMillan et al., 2014; Sevee et al., 2000; Varljen et al., 2006). For example, Varljen et al. (2006) formulated a model to calculate the flow rate through screen at steady state, and it was found that the aquifer heterogeneities had the most significant influence on the actual monitoring zone, while the pump placement and purging rate had little influence on the vertical interval that was sampled. McMillan et al. (2014) found that when the method of low-flow purging was applied, the purging rate may not always be sufficient to overcome vertical flows in wells driven by ambient vertical head gradients. While these studies have provided important scientific basis for the interpretation of groundwater sampling data, they have provided limited help to professionals who struggle to comply with regulatory guidance (Barcelona et al., 2005).

The present study intends to use a numerical model to better simulate groundwater flow during sampling for the two most widely used sampling methods: the low-flow purge method and the three well-volume method (USEPA, 2002). This new model may better represent the real situation because it incorporated the groundwater flow equation with one-dimensional advection-dispersion transport equation to describe the in-well flow. Moreover, the model accounted for water flow in sampling tubing and measurement flow chamber. Field data collected from two groundwater monitoring wells, one applied the low-flow purge method, and the other applied the three well-volume method, were used to test the validity of the model. The numerical model formulated in this paper allows professionals to optimize groundwater sampling in several aspects: 1) what is the effect of various purging on well drawdown and groundwater representativeness; 2) what water quality parameter is the most useful in ensuring representative sampling; 3) what site characteristics (e.g. aquifer permeability, water depth) will affect sampling process and how to optimize sampling strategies under various site conditions; and 4) what sampling choices (e.g. purging rate, well size, screen length) will affect sampling process and what are the optimum choices.

2. Methods

2.1. Conceptual model of groundwater flow during groundwater purging

The conceptual model of groundwater flow during groundwater purging was shown in Fig. 1. When the method of three well-volume purging was applied, an electric submergible pump was used. The in-well water was pumped through tubing to a flow chamber, and the detector was installed in the flow chamber to measure water quality parameters (DO, pH, specific conductance, temperature, ORP and turbidity). When the method of low-flow purging was applied, a peristaltic pump on the ground was used, and only tubing was inserted into the well.

When pumping a monitoring well, the pump effluent originates from four distinct sources: water in the casing interval, screened interval and tubing before purging commences, and water in the aquifer that flows into the screened interval during pumping (formation water). Usually the casing water was deemed as unrepresentative water, because water at top of the well would be influenced by the atmosphere, and water quality parameters and contaminants had a potential stratification through the well (Chatelier et al., 2011; McDonald and Smith, 2009; Pauwels et al., 2015). The formation water was in the aquifer and was able to represent the groundwater quality. However, it remained uncertain whether the water in the screen portion could represent the quality of groundwater. The method of "passive sampling" supported the idea that the screen water could represent the groundwater at equilibrium flow conditions, and the validity of passive sampling had been proved in detecting nonvolatile constitutes, heavy metal and pesticides (Berho et al., 2013; Britt et al., 2010). In this study, when the method of low-flow purging was applied, only tubing would insert into well water and therefore screen water was still considered representative of formation water. However, the installation of electric submergible pump and its vibration in the purging process would cause fierce mixing of well water when the method of three well-volume purging was applied, so the screen water would no longer be representative in this situation.

2.2. Groundwater flow equation

The governing equation for saturated flow through porous media is given by Eq. (1), which was developed from the fundamental principle of mass conservation (continuity equation) and Darcy's law (Bear, 1972):

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial z}(K_z\frac{\partial H}{\partial z})+W=S_s\frac{\partial H}{\partial t} \tag{1}$$

where K_x and K_y are hydraulic conductivity values in the x and y directions (m/s); K_z is the vertical hydraulic conductivity value in the z direction (m/s); H is the total hydraulic head (m), S_s is the specific storage of soils or water (m^{-1}); t is the time (s); W is the source/sink at every cell (s^{-1}), and it could be calculated by the following equation:

$$W=\begin{cases}-\frac{Q}{V_{pump}}, & \text{at the pumping cell}\\ 0, & \text{others}\end{cases} \tag{2}$$