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A Re-Circulating Tracer Well Test method for measuring reaction rates in fast-flowing aquifers: Conceptual and mathematical model

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SUMMARY

Reactive groundwater tracer tests provide a practical means by which rates of reaction processes that constitute natural attenuation can be measured in aquifer systems. We present a two-well Re-Circulating Tracer Well Test (RCTWT) method that we conceive applicable to determining in situ reaction rates in fast-flowing alluvial aquifers where conventional small-scale single-well tracer tests, such as the push–pull test, might be impractical. The RCTWT concept was analysed mathematically and breakthrough curve datasets were generated using a numerical model to simulate hypothetical aquifer systems from which the sensitivity of the RCTWT method to governing mathematical variables was analysed. A simplified data interpretation method for determining reaction rates from observed RCTWT breakthrough data was developed. It was demonstrated that the efficiency of the RCTWT is strongly affected by the degree of aquifer heterogeneity and the performance can be optimised by applying a high pumping rate along with a short doublet well-spacing. The simplified method provided reasonably accurate estimates of first-order reaction rate coefficients when evaluated using the hypothetical datasets, from which it was concluded that the RCTWT is a valid concept for determining potential in situ reaction rates. The findings are to be incorporated in the design of practical RCTWTs aimed at measuring denitrification rates in fast-flowing alluvial aquifers, in New Zealand.

Introduction

Reactive groundwater tracer tests provide a practical means by which rates of reaction processes such as retardation and biodegradation, that constitute natural attenuation processes, can be measured in aquifer systems. Such rates are often sought for groundwater pollutants on a site-specific basis, for the purposes of risk assessment and groundwater resource management. The basis of a reactive tracer test is to study the fate of both a conservative and a non-conservative (reactive) groundwater tracer in situ. A time-series evaluation of tracer concentrations is made from measurements taken at one or more groundwater observation wells. The reactive tracer usually comprises a groundwater pollutant of concern, or a reagent or product of a specific chemical or biological reaction process being investigated. The conservative tracer dataset is used to characterise transport phenomena, e.g. dilution and dispersion processes, and provide a reference against which the reactive tracer data are compared. Reaction rates are subsequently calculated from the rate at which the observed reactive tracer data record deviates from the record that would have been predicted based on transport processes alone.

The single-well push–pull test (Istok et al., 1997) is probably the most commonly applied small-scale reactive tracer test used for determining rates of in situ reaction processes (e.g. Schroth et al., 1998; McGuire et al., 2002; Istok et al., 2004). The push–pull test offers a practical and economical alternative to the approach of conducting large-scale natural gradient tracer tests using multiple wells (e.g. Smith et al., 2004). An added appeal of the push–pull test to groundwater practitioners is the availability of simplified analytical data interpretation models (Haggerty et al., 1998; Snodgrass and Kitanidis, 1998) that avoid the need to process test data using complicated numerical models.

Both natural gradient and single-well reactive tracer tests are subject to practical limitations in aquifer settings where tracer reaction is slow relative to the natural groundwater velocity. Slow reacting tracers require a long residency in the aquifer before concentrations alter a measurable amount. For the natural gradient tracer test this implies monitoring must be conducted over a long distance of the natural flowpath. With this increase in scale is associated an increase in practical costs that may become prohibitive. Similar scale issues apply to the push–pull test, in which a reactive solute is injected and recovered from a single well. In a push–pull test the injected tracer solution will drift from the test well once injection is completed and, with time, drift beyond the zone of

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recapture (Bear and Jacobs, 1965). The only practical means of increasing residence time of the tracer (as might be required if reactions are slow) is to scale up the test by increasing both the pumping rate and volume of reactive solution that is injected into the aquifer (Bear and Jacobs, 1965). If the regional groundwater velocity is fast, a large volume of tracer solution may be required that could prove impractical. Burbery et al. (2004) provide an example of a field push–pull test conducted in a fast-flowing aquifer, the outcome of which was poor tracer mass recoveries that contributed to large uncertainties in the data interpretation.

One way to improve hydraulic control of solute injected into an aquifer (thereby improve tracer mass recovery) is to employ a two-well, forced-gradient tracer test. This style of test has traditionally been used in the past to characterise flow and transport properties of aquifers (e.g. Webster et al., 1970; Molz et al., 1986). Ptak and Schmid (1996) and Hoehn et al. (1998) applied this type of test to the study of retardation of groundwater solutes. More recently, re-circulating well schemes have been used as engines for in situ treatment of contaminants in the field of groundwater remediation (McCarty et al., 1998; Ryan et al., 2000; Cunningham and Reinhard, 2002; Gandhi et al., 2002; Luo et al., 2006). Re-circulating water between two wells effectively extends the residence time of water within the local system. To the best of our knowledge, two-well schemes have never been used as a device for directly determining in situ reaction rates, although developments have been made on adapting the single-well (vertical) dipole flow tracer test for measurement of reaction rates (Reiha, 2006). We envisage that a two-well, Re-Circulating Tracer Well Test (RCTWT) might be applied to estimate reaction rates, such as those of microbial respiration, in situ, in fast-flowing contaminated aquifers, where application of the single-well push–pull test might be impractical. As a practical concept, the RCTWT fits between the physical and economic scales of the single-well push–pull test and large-scale multi-well tracer tests. A focus of this paper is to outline details of the RCTWT concept.

Prior to its application, it is necessary to analyse the performance of the RCTWT as affected by various physical and environmental factors through mathematical modelling so that the findings can be incorporated into the design of practical tests. Mathematical analysis of the RCTWT forms an objective of this paper. In the past, the performance of two-well forced-gradient tracer tests has been evaluated using mathematical models that either do not account for the effects of hydrodynamic dispersion (DaCosta and Bennett, 1960; Grove et al., 1970; Datta-Gupta et al., 1995; Zhan, 1999; Luo and Kitanidis, 2004) or which assume the absence of a regional flow field (e.g. Grove and Beetem, 1971; Welty and Gelhar, 1994; Koplik, 2001; Constales et al., 2003). Here, we present a full mathematical model that describes the flow and transport processes under the RCTWT in aquifers with fast regional groundwater flow. The most important factors affecting the performance of the RCTWT are analysed using numerical simulations with finite elements.

The final objective of this paper is to develop a simplified data interpretation method for determining reaction rates from RCTWT tracer breakthrough curves (BTCs). The accuracy of this simplified method is evaluated by comparing estimated reaction rates, obtained by the simplified method using BTCs generated by numerical simulations, with actual reaction rates that were used in numerical simulations.

Conceptual model of the RCTWT

Our research has primarily been driven by a need to develop a practical method for measuring denitrification rates in fast-flowing, alluvial aquifers, in New Zealand. It is for this reason that we shall illustrate our concept with a focus on measuring nitrate reaction rates, although the principles of the RCTWT are not exclusively limited to nitrate contamination. Here we describe the conceptual model of the RCTWT in terms of the four principal stages of practical implementation. We also outline some underlying assumptions.

Stage 1: the physio-chemical problem

Consider an aquifer that is extensively impacted by a nitrate plume. Denitrification serves as the only sink of nitrate, albeit reaction is slow relative to the velocity of contaminant transport in groundwater. As a consequence, under natural conditions, reductions in nitrate concentrations along the flowpath are only measurable over a large distance. It is beyond the scope of this study to evaluate the implications of specific biogeochemical variables (e.g. oxygen and substrate availability, and microbial biomass) that control denitrification, and so we shall assume that denitrification in the conceptual system is effectively rate-limited and follows a first-order reaction process. This simplifying assumption is not uncommon in contaminant modelling where non-linear, even multifunctional reaction kinetic parameters are often lumped into a single effective rate constant (Bekins et al., 1998; Aronson et al., 1999). Moreover, first-order rate constants are generally an adequate descriptor of biodegradation rate processes in situations where reagent concentrations are low and biomass is constant (Simkins and Alexander, 1984). The local hydraulic gradient of the aquifer in the vicinity of the test site is assumed known and is relatively uniform. An effective reaction rate is sought for the nitrate pollution.

Stage 2: doublet well set-up

Employing the concept that maximum interflow is obtained when a well-pair is orientated parallel with the direction of the regional groundwater flow (DaCosta and Bennett, 1960), two wells are installed along the regional groundwater flow direction (Fig. 1). From a practical perspective, this requirement alone restricts the RCTWT application to situations where aquifer flow conditions have been characterised in advance. In the absence of any additional monitoring wells in the local vicinity of the test, the initial test conditions, namely, background tracer concentrations, are measured from the installed doublet wells. We conceive that because of the relatively small scale of the doublet scheme (and short

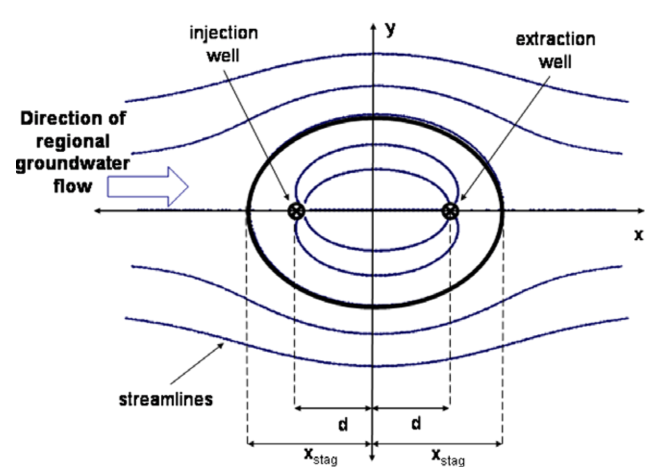

Fig. 1. Example of RCTWT geometry in a homogeneous confined, isotropic aquifer. Parameters are described in the text. Bold ellipse marks the extent of the dipole flow cell – theoretical stagnation points in mathematical model.