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Using predictive uncertainty analysis to optimise tracer test design and data acquisition

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SUMMARY

Tracer injection tests are regularly-used tools to identify and characterise flow and transport mechanisms in aquifers. Examples of practical applications are manifold and include, among others, managed aquifer recharge schemes, aquifer thermal energy storage systems and, increasingly important, the disposal of produced water from oil and shale gas wells. The hydrogeological and geochemical data collected during the injection tests are often employed to assess the potential impacts of injection on receptors such as drinking water wells and regularly serve as a basis for the development of conceptual and numerical models that underpin the prediction of potential impacts.

As all field tracer injection tests impose substantial logistical and financial efforts, it is crucial to develop a solid a-priori understanding of the value of the various monitoring data to select monitoring strategies which provide the greatest return on investment.

In this study, we demonstrate the ability of linear predictive uncertainty analysis (i.e. "*data worth analysis*") to quantify the usefulness of different tracer types (bromide, temperature, methane and chloride as examples) and head measurements in the context of a field-scale aquifer injection trial of coal seam gas (CSG) co-produced water. Data worth was evaluated in terms of tracer type, in terms of tracer test design (e.g., injection rate, duration of test and the applied measurement frequency) and monitoring disposition to increase the reliability of injection impact assessments. This was followed by an uncertainty targeted Pareto analysis, which allowed the interdependencies of cost and predictive reliability for alternative monitoring campaigns to be compared directly.

For the evaluated injection test, the data worth analysis assessed bromide as superior to head data and all other tracers during early sampling times. However, with time, chloride became a more suitable tracer to constrain simulations of physical transport processes, followed by methane. Temperature data was assessed as the least informative of the solute tracers. However, taking costs of data acquisition into account, it could be shown that temperature data when used in conjunction with other tracers was a valuable and cost-effective marker species due to temperatures low cost to worth ratio. In contrast, the high costs of acquisition of methane data compared to its muted worth, highlighted methanes unfavourable return on investment. Areas of optimal monitoring bore position as well as optimal numbers of bores for the investigated injection site were also established.

The proposed tracer test optimisation is done through the application of common use groundwater flow and transport models in conjunction with publicly available tools for predictive uncertainty analysis to provide modelers and practitioners with a powerful yet efficient and cost effective tool which is generally applicable and easily transferrable from the present study to many applications beyond the case study of injection of treated CSG produced water.

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1. Introduction

Tracer injection tests are regularly-used tools to identify and characterise flow and transport mechanisms in aquifers. Such tests

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can be used to derive subsurface hydraulic properties, and to investigate the transport behaviour of both non-reactive and reactive solutes in groundwater. Examples of practical applications are manifold and include, among others, managed aquifer recharge schemes (e.g. Culkin et al., 2008; Descourvieres et al., 2010; Wallis et al., 2011), aquifer thermal energy storage systems (e.g., Zuurbier et al., 2013), the storage of CO_2 emissions in deep aquifers (e.g. Michael et al., 2010) and, increasingly important, the disposal of treated coals seam gas (CSG) production water or produced water from oil and shale gas wells into deep aquifers (NWC, 2011; U.S. Dep. of the Interior, 2011). The hydrogeological and geochemical data collected during the injection tests often serve as a basis for the development and parameterisation of conceptual and numerical models that are subsequently used to predict the larger-scale and longer-term hydraulic and water quality impacts of operational injection, storage and abstraction schemes.

All field tracer injection tests impose substantial logistical and financial efforts. This is particularly so within the context of injection of CSG-produced water, given the often considerable depth of the targeted aquifers, in many cases exceeding 1 km. A significant number of sampling events is often not only required during injection, especially under dynamically changing flow conditions, but also in the post-injection monitoring phase, to capture long-term geochemical changes. Monitoring may include continuous recording of various data types using cost-effective down-hole sensors, for example for temperature, pressure or electrical conductivity data (Ma et al., 2012). However, data acquisition for most chemical constituents to date still relies on more costly laboratory analysis of water samples. To minimise efforts and costs, sampling strategies that can most efficiently identify and characterise the transport mechanisms and geochemical processes in the targeted aquifers within the given budget and access constraints need to be chosen. A robust a priori understanding of the costs and the value (i.e., data worth) of the available data types will allow (i) optimisation of the trial design (e.g., types of tracers amended, concentrations of amended tracers, duration of amendment); (ii) optimisation of monitoring strategies (e.g., type and frequency of the collected data); and (iii) reduction of the uncertainty of model predictions, and thus maximise the predictive power of models simulating long-term impacts during and after operational injection. The proposed methodology requires to set up a numerical groundwater model already ahead of the trial.

Within the context of water resources modelling, the assessment of "*data worth*" involves quantification of the utility of observation data in reducing the uncertainty of model predictions of future environmental behaviour (e.g., first or mean contaminant arrival time, magnitude of plume spreading) which underpin management decisions. The value of a data type or an observation location is greater, the more it enhances the certainty with which the model is able to predict such environmental behaviour. By comparing the difference in predictive uncertainty with or without such data, the value of potential observations is assessed. Predictive uncertainty is typically computed using global optimisation methods, such as Monte Carlo simulations (e.g. James and Gorelick, 1994; Parker et al., 2010; Fu and Gómez-Hernández, 2009). Monte Carlo techniques often pose a considerable computational burden, as they consist of performing a large number of forward model runs based on a random selection from model parameter distributions. Their application therefore remains restricted mostly to groundwater models of limited run-time. In order to assess data worth within the context of field-scale, multi-species non-reactive as well as reactive transport problems, where model run times and the number of adjustable parameters can be high, a computationally more efficient approach is desirable. A methodology which is applicable to field-scale problems was initially presented by Moore and Doherty (2006) and later extended by Christensen and Doherty (2008). This analysis is based on linear predictive uncertainty analysis formulated for distributed parameter models and is incorporated as the freely-available prediction uncertainty tools PREDUNC and PREDVAR into the PEST suite (Doherty, 2010a,b) (Fig. 1). The approach derives estimates of simulated prediction uncertainty based on direct propagation of uncertainties originating from incomplete knowledge of model parameters. Computational efficiency is gained by assuming that the system response is sufficiently linear over the range of evaluated parameters to establish relative contributions to uncertainty. This allows the calculation of predictive uncertainty to be made rapidly, so that it can be repeated for many alternative monitoring strategies (potential monitoring sites, potential observation data types and sampling times).

The methodology has been successfully applied to several synthetic numerical groundwater model problems. Moore (2005), for example, investigated the worth of spatially distributed head and hydraulic conductivity measurements with respect to the reliability of contaminant transport predictions. Dausman et al. (2010) investigated the relative worth of salinity and temperature observations for predictions of the location of a theoretical salt water–fresh water interface, while Fienen et al. (2010) used prediction uncertainty analysis to explore its use in a hypothetical water-level monitoring network design by analysing the worth of head measurements for drawdown and flux predictions. A recent example of the practical application of data worth to a field-scale problem was presented by Engelhardt et al. (2013), where the suitability of the artificial sweetener acesulfame as conservative tracer for sewage related fluxes and its value in constraining simulated water and mass-fluxes was investigated. Nevertheless, a wider range of studies which demonstrate the robustness of this methodology to field-scale problems in hydrogeologically and geochemically heterogeneous porous media is still lacking, and moreover, its use in conjunction with minimising the actual cost of data acquisition has also not been demonstrated. This allows for the evaluation of a monitoring strategy subject to both cost and rigour constraints and is of particular importance in the water resources context, where monitoring is typically a significant effort and often under public scrutiny.

In this study, we demonstrate the ability of linear predictive uncertainty analysis (hereafter simply referred to as "*data worth* analysis") to quantify the usefulness of different tracer types and head measurements in the context of a field-scale aquifer injection trial of CSG co-produced water. Data worth is evaluated in terms of the degree to which chemical concentrations, temperature and head data increase the reliability of injection impact assessments, employing the metrics of dilution and time of travel. The relative merits of different tracer test designs are explored. These differ in terms of where and when tracer concentrations are collected, the injection rate and duration of the test, the tracer concentration to ambient concentration ratios (signal to noise ratios) and the applied measurement frequency. We then formulate the trade-off between the established relative value of tracer data on the one hand and the costs of its acquisition on the other hand (Fig. 1) to select monitoring strategies which provide the greatest return for investment.

2. Data worth methodology

The uncertainty analysis theory underpinning the methodology of data worth is briefly summarised here to provide the theoretical background for this work. Various particular aspects are presented in more detail elsewhere (Moore and Doherty, 2005; Christensen and Doherty, 2008; Dausman et al., 2010; Fienen et al., 2010; Moore et al., 2011; Engelhardt et al., 2013).

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