Presentation Abstracts

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The Path from Data to Decisions

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Post-2009: A PEST Odyssey – Randy Hunt, USGS

Many things have changed since the first PEST conference in 2009. Much progress has been made in areas such as software capabilities and suggested practices. However, within the rapid pace of wide-ranging problem solving, developing the "hydrosense" needed to efficiently decompose modeling problems remains difficult to attain despite (and perhaps due to) the increased wealth of tools and computational capabilities. At the same time, decision-makers' needs and societal contexts continue to evolve. The result is perhaps less practical progress than might be expected given the academic advances since 2009. Yet, consideration of things learned – before and since 2009 – can provide direction for future investments of teaching and technology. Some candidate areas will be discussed in this talk.

Applying PEST++ and Iterative Ensemble Smoothing to Evaluate the Likelihood of Alternative Conceptual Models for Tailings Seepage – Michael Gabora, FloSolutions

Modern uncertainty analysis techniques present an opportunity to provide tailings engineers and decision makers with an improved understanding of hydrogeological risks for Tailings Storage Facilities (TSFs), and by extension, actions or design changes that can reduce those risks. A key objective of this study is to evaluate the likelihood and viability of two alternative conceptual models to explain the measured hydraulic heads and fluxes, and perhaps, provide insights into additional hydrogeologic parameterizations that may explain observed conditions.

Inverse modeling techniques available in PEST++, namely Iterative Ensemble Smoothing (IES), is applied to forecast seepage fluxes and flow paths from a large conventional TSF. A highly parameterized MODFLOW-USG model was developed and calibrated to more than 15-years of historical measurements for heads, spring discharge, water balances and seepage fluxes to embankment drains. The resulting history match constrained, stochastic parameter fields are interrogated to provide insights on the validity and likelihood of the working conceptual models. This assessment is key for understanding how seepage flow has changed through time, particularly given the understanding that the highly dynamic system that includes saturation of previously unsaturated materials, regular embankment raises, and many other operational and water management changes.

This case study provides lessons learned regarding model structural complexity and numerical nuances of IES, which are particularly important considering that many aspects of operational TSFs complicate modeling and history-matching efforts. Complicating factors include, (1) the need for resolving vertical gradients in high-resolution, (2) transient processes associated with embankment raises, (3) changes in liner and internal drain configurations, (4) sedimentation and consolidation of tailings, (5) highly variable toe drain and well pumping rates, (6) changing hydraulic properties through time, and so on. As a result, decisions around suitable compromises and simplifications can be difficult given how sensitive many of these complexities are on model forecasts. Case study results are focused on the viability of various conceptual models and other potentially viable concepts of seepage flow elucidated by the ensemble analysis.

Forecasting Future Groundwater Levels in the Mississippi Delta Region, USA, Andrew Leaf, USGS Upper Midwest Water Science Center – Andrew Leaf, USGS Upper Midwest Water Science Center

The Mississippi Delta is a productive agricultural region encompassing ~7,000 mi 2 of alluvial floodplain between the Mississippi and Yazoo Rivers in northwest Mississippi, USA. Important crops include soybeans, corn, cotton, rice and aquaculture (catfish), with a total economic impact of ~$3 billion. Irrigation from the alluvial aquifer to offset high rates of evapotranspiration in a subtropical climate has resulted in groundwater

declines of 15 meters or more over the last century. Recent wetter than average conditions have stabilized groundwater levels somewhat, but future trends are unclear. Stakeholders are interested in forecasts of future groundwater levels under varying climate and groundwater management scenarios.

Using MODFLOW 6, Soil Water Balance Code and several open-source python packages, the USGS Mississippi Alluvial Plain Study created a hydrologic model that incorporates the terrestrial water balance, metering-based estimates of water use from thousands of wells, measured and estimated stream flows and stages, and the largest airborne electromagnetic (AEM) survey flown to-date in the United States. History matching for parameter estimation was performed with PESTPP-IES (iES). A fully-scripted workflow with version control was used to add or subtract features from the model structure and parametrization in response to successive iES runs. The selected model configuration employed 56,730 adjustable parameters representing scales ranging from individual stream reaches (at the km scale), to model or dataset-wide multipliers. Parametrization was implemented using the automated PstFrom framework in pyEMU. 10,980 weighted observations included measured heads and total stream flows, as well as derivative observations such as temporal and spatial differences and linear head trends. Despite a large number of parameters and relative abundance of data, there were many challenges to history matching. Although the AEM survey provided semi-quantitative information about the relative hydraulic conductivity (K) structure of the highly heterogeneous alluvial aquifer, absolute values of K were sparse, and incorporation of 5-meter (vertical) resolution AEM data led to 21 model layers. Total streamflows were mostly well-matched, but a small groundwater component (~10% of total streamflow) made it difficult to constrain groundwater fluxes, especially recharge. Simulation of total streamflow allowed for accurate representation of groundwater/surface water gradients, especially under future climates, but came at the cost of increased model runtime. Finding the right balance between fine and coarse-scale parametrization, and the "right" parameter structure required extensive trial-and-error. Knowledge of the extent and relative thickness of a shallow confining unit from the AEM survey proved useful for parametrizing recharge. Results indicate a complex water balance that varies in time and space in terms of the terrestrial recharge, stream leakage and regional groundwater flow components, which are influenced by seasonal forcings, human activity and alluvial geomorphology. The terrestrial water balance allows future climate scenarios to consider potential climate-driven changes to irrigation abstraction, groundwater recharge, and streamflow. With iES, model uncertainty can also be easily considered. The model construction and parameter estimation workflow is designed to facilitate regular updating, making this a "living" framework that stakeholders can use for adaptive management going forward.

Groundwater Objective Analysis Tool – A Tool for Predictive Management of Groundwater Substitution Program in Yuba Basin – Sercan Ceyhan, Woodward & Curran

The Yuba Water Agency (Yuba Water) promotes the beneficial conjunctive use and sustainable management of the surface and groundwater resources of the Yuba Watershed in collaboration with its Member Units; local, state, and federal agencies; and other stakeholders. Yuba Water's efforts benefit the residents of Yuba County and residents in other parts of the state through sustainable groundwater conditions and water transfers. To date, Yuba Water Member Units have provided over 600,000 acre-feet of surface water to users across the state through groundwater substitution transfers. Yuba Water uses a series of predictive management tools using real-time data, modeling, and economic indicators to inform the Member Units during the decision-making process for one or more years of groundwater substitution pumping to limit short-and long-term impacts from groundwater pumping. One of the predictive management tools is the Groundwater Objective Analysis Tool. This tool uses the Yuba Groundwater Model (YGM) and PEST to simulate an ensemble of hydrologic and pumping conditions to inform management decisions on the annual volume of groundwater substitution pumping. This presentation will focus on the development of the Groundwater Objective Analysis Tool and the technical details of the analysis. We will talk about the PEST setup that runs YGM and the pre-processing and post-processing routines, present results, and talk about the future of the tool.

(INVITED) Reflections on Model Calibration, Uncertainty Analysis, and Forecasting – Greg Ruskauff, INTERA Incorporated

Modeling can be a powerful tool to help make decisions. Pitfalls include having sufficient data of the right kind to understand the system (and interpreting it correctly) and formulate a correct conceptual model, not to mention parameterizing a model to usefully represent reality. Examples of the importance of conceptualization and how the parameter estimation framework can help will be discussed, as well as when it can't. Uncertainty analysis is also a powerful way of assessing the risk associated with a decision, and examples will be discussed. In the end, the computer can't be relied upon to generate the answer (even IES), and thinking is required!

Quantifying Groundwater Model Uncertainty in Urban Environments - Innovative Techniques for a Challenging Task – Kevin Hayley, Groundwater Solutions Pty Ltd

The modelling of groundwater flow and transport in urban environments is complicated by recharge alterations and interaction with water supply and sewer infrastructure. This study presents an attempt to capture the complexity and quantify the uncertainty of groundwater flow and mass transport in urban environments using new methods. The study site was an industrial plant with historical groundwater contamination. Remediation had been conducted at the site over 12 years to excavate the impacted soil install a groundwater pump and treat system. Groundwater flow and mass transport modelling was required to evaluate the risk of adverse impacts upon a nearby creek if the pump and treat remediation system was discontinued. A python scripting approach was used for model development and the setup of a calibration constrained parameter uncertainty analysis using the iterative ensemble smoother method (IES). Water supply and sewer infrastructure locations were directly included in the model as boundary conditions. The model calibration considered more than 100,000 independent parameters, applied at zones, pilot points and directly on the model grid to define model properties, boundary conditions, and initial conditions. Calibration observations included both water level and concentration measurements at boreholes over the 12-year operational life of the remediation system. The IES method was applied to calibrate 120 alternative and equally plausible parameter realizations, which were produced from initial statistical distributions defined by reasonable parameter bounds and spatial correlation. The Amazon EC2 cloud computing service was used to provide the parallel computing capacity necessary to complete the project in a short timeframe. Predictions of long-term mass transport towards the creek were made with each of the resulting parameter sets. The method provided a distribution of potential impacts and allowed any decisions concerning the future of the current pump and treat system, to be made based on a quantitative, statistical, risk- analysis.

Computationally Efficient Hypothesis Testing Using an Iterative Ensemble Smoother and Reproducible Workflows – Guillermo Martinez, PhD, PE, INTERA Incorporated

Many of the environmental challenges we face as a society require the use of numerical models to evaluate potential undesirable conditions using limited data and imperfect representation of natural and human systems. Iterative ensemble smoother (IES) methods are a computationally efficient and robust approach to evaluate the uncertainty of numerical models and the worth of adding additional observation sources. IES methods also provide a way to test hypotheses about modelling assumptions and conditions in problems often too complex for traditional statistical methods.

This work presents an approach to test hypotheses on undesirable outcomes in complex decision support models by taking advantage of the efficient and parallel capabilities of IES methods. The model used to illustrate the approach represents a groundwater system with around 200 observation points and more than 70,000 parameters to describe hydraulic properties and boundary conditions. The version-controlled workflow used to implement the uncertainty analysis and hypothesis testing meticulously documents each step of the

analysis and takes advantage of open-source libraries to manipulate model files, implement the ensemble methods, and efficiently evaluate the fate of a contaminant of concern. After a careful evaluation of conflicts between prior parameters and observations, the prior parameter ensemble is updated by IES to improve the match between simulations and observations. Historical observations were augmented with a spatial metric representing the condition where the hypothesis could be accepted.

Results of the analysis illustrate the trade-off between fitting observations and the hypothetical undesirable outcome as well as the impact on parameter value plausibility. The computational performance and flexibility of this approach provides a robust, efficient, and reproducible decision-support modelling tool for solving mining and environmental challenges.

Reproducible Parameter Estimation Framework for Integrated Hydrological Models – Seonggyu Park, Texas A&M AgriLife Research

A recent version of the Agricultural Policy / Environmental eXtender (APEX) model integrates the physically-based, spatially distributed groundwater flow model MODFLOW. The integrated model code was extended to simulating nutrient and salt ion transport. We developed a reproducible optimization framework for the integrated APEX-MODFLOW-RT3D-Salt (AMRS) model, to assess sensitivity analysis (SA), uncertainty quantification (UQ), and parameter estimation (PE). A case study was conducted in the Animas River watershed, which spans portions of Colorado and New Mexico, USA. A script-based workflow, a Python package called apexmf, is developed for use with the interactive Jupyter notebooks and for increasing the credibility of the AMRS model as a decision tool. In the case study, a total of 123 significant parameters, such as soil moisture retention parameter, initial abstraction, Hargreave's PET coefficient, hydraulic conductivity, specific yield, riverbed conductance, riverbed thickness, were assigned as field and boundary parameters. A high-dimensional PE was performed to reduce uncertainty through comparing monthly average simulated and observed streamflow discharges and daily groundwater levels. Streamflow discharges were compared at four different locations during 1992-2011, and groundwater levels from two observation wells were used.

Numerical Simulation of Remedial Alternatives for a Chlorinated Volatile Organic Compound and 1,4 Dioxane Plume – Dave Estrella, AECOM

A numerical groundwater flow and contaminant fate and transport model was developed to evaluate remedial alternatives including dual-phase extraction at the source area and monitored natural attenuation and pump and treat in the downgradient wetlands for chlorinated volatile organic compounds (CVOCs) and 1,4-dioxane plumes originating from a manufacturing facility. The numerical model was constructed with MODFLOW-USG Transport [1, 2] using the pre- and post-processor Groundwater Vistas Version 8 [3]. The model mesh was generated using AlgoMesh 2 [4]. The PEST software suite was utilized for model calibration [5, 6]. Additional pre- and post-processing was performed in ArcGIS version 10.8 [7].

Initially, a three-dimensional steady-state groundwater flow model was developed and calibrated to average water levels from 2015 through 2021 as well as flow directions from groundwater contours maps and CVOC and 1,4-dioxane dissolved phase concentration distribution patterns using particle tracking with mod-PATH3DU [8]. Pilot points and Singular Value Decomposition-Assist (SVD-Assist) were tools that were used within the PEST software [9]. Then, the calibrated steady state flow model was converted to a transient flow model to simulate the timeframe beginning with the reported release in 1970 and ending with current conditions. Variable pumping rates of a groundwater extraction and treatment system were incorporated during the time of operation from 1995 to 2001.

Fate and transport of CVOCs and 1,4-dioxane were simulated using the transient groundwater flow model assuming a constant source term and incorporating dispersion, sorption, and degradation as attenuation factors. The constant concentration source zone was conceptualized based on the stable trends of dissolved

phase concentrations in the area of suspected dense non-aqueous phase liquid (DNAPL). Calibration of the fate and transport model included iterative adjustments of transport parameters and the groundwater flow model parameters until the simulated concentrations achieved an acceptable fit to observed concentrations in groundwater, interpreted plume distributions, and measured outflow concentrations from the groundwater extraction and treatment system effluent.

Predictive simulations compared simulated concentrations in the wetlands to applicable regulatory standards. First, natural attenuation was simulated to predict maximum concentrations in the downgradient wetlands in the absence of any active remediation. Then, separately the proposed dual phase extraction system was evaluated, assuming that it would remove the suspected DNAPL source within 10 years. Finally, groundwater pump and treat strategies in the wetlands were simulated and considered in conjunction with dual phase extraction.

To evaluate the effects of model assumptions on predictions and outcomes, a sensitivity analysis was performed on model inputs. Select parameters were varied within appropriate ranges based on field data and literature values, assessing the potential uncertainty and variability of predictions. This modeling effort allows stake holders to make decisions about remedial strategies in the context of the local regulatory framework and in keeping with the client's strategy and budget.

Coupling a Recharge Estimation Model with a Groundwater Flow Model to Improve Environmental Management Decision Support for Mining Operations – Savannah Miller, Brown and Caldwell

Coupling a recharge estimation model with a groundwater flow model to improve environmental management decision support for mining operations. Advances in groundwater modeling software have enhanced the use of groundwater models for hydrologic decision support systems. The development of groundwater models using versions of MODFLOW 2005 and prior, are labor intensive due to data input structures, nuanced hydrologic input packages, serial processing, and many other factors. The time requirement of historical groundwater models inhibited their application in complex projects such as mine operation impact evaluations where numerous scenarios are needed.

In recent years, the release of MODFLOW 6, and the python package FloPy, have allowed for many pre- and post-processing tasks to be automated and parallelized. These advancements allow modelers to streamline workflow, allow for more robust testing and promote comparative analysis of groundwater model results for multiple scenarios. MODFLOW 6 also incorporates local grid refinement which provides higher resolution results in areas of interest with minimal impact to total model run times. With these advancements, groundwater modeling can now be a more effective contributor to project decision support at mine sites because of improved ability to evaluate model uncertainties.

With a more efficient groundwater modeling workflow, coupling other hydrologic models to the groundwater model is easier to implement. This case study illustrates coupling a modified Thornthwaite-Mather runoff estimation model from the USGS (Soil-Water-Balance (SWB)) with a MODFLOW 6 groundwater flow and transport model for a mining client in support of the NEPA process. The coupling of the SWB and MODFLOW 6 model results in a rapid, repeatable, and robust method to assess climate change impacts, land use alterations, and mining activity impacts on groundwater and surface water resources during mining operations.

Case Study – Ensemble Smoother to Support Decision-Making Process – Mark Ranjram, Matrix Solutions Inc.

This presentation will look at a series of case studies where PESTPP-iES (iterative ensemble smoother) was used to quantify uncertainty associated with numerical model predictions.

- Case Study #1 – Nuclear Power Plant – Potential Source Release Identification – France

- Case Study #2 – Hydraulic Capture Optimization for Groundwater Treatment Plant Design – Quebec, Canada
- Case Study #3 – Probability of Chloride Impacts to Future Residential Water Supply Wells – Alberta, Canada
- Case Study #4 – Uncertainty in Groundwater Flow Direction – California, United States

The objectives, purposes, outcomes, challenges, and particularities from each case study will be briefly discussed, with a focus on the ensemble smoother implementation. Hydrogeological material properties and/or spatial distribution of hydro-facies was conducted using different approaches that will be discussed: multiple-point statistics (MPS), sequential gaussian simulation (SGS), zonation, and pilot points.

Scientist can always improve how they convey results from uncertainty analysis to decision-makers. One of the common challenges in the case studies presented was to synthetized results so that the outcomes are clear to non-modellers. Results communication will be discussed throughout the presentation.

Finally, one of the most difficult conundrums we've experienced was how to conduct knowledge transfer? Model files, custom programs/scripts, workflows, computing environment and computational resources availability can all contribute to challenges in knowledge transfer. Based on author's experience, data science tools can be useful, but clearly defined expectations at project's initiation are paramount to effective knowledge transfer.

Capture Zone Analysis for Deep Groundwater Plumes: Addressing Uncertainty using Multiple Lines of Evidence – Michael Rush, Neptune

Capture zone analysis can be used to understand the performance of pump-and-treat systems such as the Chromium plume interim measure (IM) at Los Alamos National Laboratory (LANL). A plume of hexavalent chromium (Cr6+) has been detected in excess of the 50 ppb New Mexico groundwater standard in the regional aquifer below LANL property in multiple monitoring wells; the highest measured concentration is approximately 1,000 ppb. Comprehensive investigations of the plume have been ongoing since 2005 (LANL 2008, 2009, 2012). The IM network, which includes five injection (CrIN) wells and five extraction (CrEX) wells, was planned and developed with the objectives of (1) maintaining a 50-ppb downgradient plume edge within the laboratory boundary and (2) hydraulically controlling plume migration in the eastern downgradient portion of the plume (LANL 2015, 2018).

Multiple, converging lines of evidence based on site data and numerical modeling are combined to most effectively evaluate system behavior and uncertainty of capture zone estimates. We first present a set of data-based methods, in which hand-contouring of synoptic water level measurements highlight differences in site hydraulics between IM system operation and baseline conditions. Next, we use numerical modeling to evaluate capture zones at the Chromium plume site. Four deterministic calibrations representing unique source terms and flow pathways are identified using a gradient descent method (all are consistent with the conceptual site model and closely match available data). This allows for more thorough explorations of uncertainty in the deep groundwater, data-poor system.

Capture zones are drawn, with uncertainty, using three different approaches that leverage the calibrated numerical model with uncertainty: a streamline analysis (2D), particle tracking (3D), and a concentration-based analysis (3D). Capture zones from different methods provide different quantitative metrics to understand system performance. These include (1) using steady-state simulations to differentiate "escaped" Cr6+, which would not be captured by the fully operational system, from "cleaved" Cr6+ that escapes the IM solely because it started its transport through the regional aquifer before the IM was fully operational; (2) Identifying particle pathways for potential escape and predicted concentrations of Chromium along these pathways; and (3) delineating zones of hydraulic influence as opposed to zones of capture.

Generally, the water level, map-based methods and streamline-based methods suggest a larger capture zone than other estimates, which include physics-based simulation of contaminant transport. Using forward particle tracking from the Chromium source locations, we identify and describe pathways for particles originating at contaminated areas to bypass the IM. We explore the nature of these paths with associated depths and concentrations from the model. Results suggest that the extraction wells reduce concentrations significantly enough within the capture zone that dispersion, diffusion, and mixing with clean sources reduces most escaped Chromium concentrations to below 50 ppb by the time Chromium is advected significantly downgradient of the IM system.

LANL, 2008. Fate and Transport Investigations Update for Chromium Contamination from Sandia Canyon, LA-UR-08-4702, EP2008-0374, Los Alamos National Laboratory, Los Alamos NM, July 2008

LANL, 2009. Investigation Report for Sandia Canyon, LA-UR-09-6450, EP2009-0516, Los Alamos National Laboratory, Los Alamos NM, October 2009

LANL, 2012. Phase II Investigation Report for Sandia Canyon, LA-UR-12-24593, EP2012-0195, ERID-228624, Los Alamos National Laboratory, Los Alamos NM, September 2012

LANL, 2015. Interim Measures Work Plan for Chromium Plume Control, LA-UR-15-23126, EP2015-0089, Los Alamos National Laboratory, Los Alamos NM, May 2015

LANL, 2018. Chromium Plume Control Interim Measure Performance Monitoring Work Plan, LA-UR-18-23082, EP2018-0055, Los Alamos National Laboratory, Los Alamos NM, April 2018

Communicating Complexities of Mathematical Models in Decision-Based Multistakeholder Negotiations – James Schuetz, PG, and Kylah Wyatt, Parsons

Mathematical models are an important tool in providing insight into complexities of a geological system, thereby supporting difficult and / or challenging decisions. Communication of complex mathematical processes is a critical component in effective and efficient decision making when implementing these tools. The importance of clear communication is highlighted in sensitive projects, such as, environmental contamination which poses real or perceived risk to the public. That said, the mathematical modeling community has, at times, struggled to provide impact to the decision making process due to ineffective communication. This problem exists for a variety of reasons including (but not limited to): software limitations, algorithm accessibility, communication skills, and lack of acceptance from stakeholders. As numerical modeling capabilities have continually improved, recent expansions in developing and communicating uncertainty provides the modeling community tools and techniques to improve how important information is conveyed. With improvements in communication, decisions can appropriately incorporate highly technical mathematical modeling while limiting miscommunication and avoiding extended negotiations.

This presentation will provide an overview of challenges in communicating mathematical modeling, techniques for improving communication and stakeholder acceptance, as well as case study examples of pitfalls and successes from a variety of projects. Classification of techniques presented will include: open and accessible modeling and code, thoroughness in reporting, understandable content, and presentation of model uncertainty. Multiple case study examples will be provided that include failures in communication of groundwater models resulting in indecision and wasted resources, examples of technical content that was poorly received and / or misunderstood, as wells as instances of successful projects where communication techniques were targeted to the audience. With PEST++ there have been significant improvements in the development and presentation of uncertainty. Project examples of numerical groundwater modeling including rise of water table conditions resulting from predicted 100 year increase in sea level will demonstrate the use of PEST++ and the abilities to effectively analyze and communicate associated uncertainties with the predictive modeling results to stakeholders to support decision making.

(INVITED) Are Decisions Better With Pest? -- A Consultant's Perspective from the Trenches - Charlie Andrews, S.S. Papadopulos & Associates

Groundwater models are constructed for many purposes, but at S.S. Papadopulos & Associates we believe the models we construct are intended to aid to decision making and to assist in better management of water resources. The tools that have been developed over the past 40 years, since I started my career, to assist in model construction, model calibration, and model use are awesome. Without a doubt, current models can provide better forecasts than previous models to assist in decision making. These better models though can have significant time and money costs. In this talk I will examine, based on case histories, the decisions clients need to make, how we have used groundwater models to support the client in decision making, and how the use of groundwater models for this purpose has changed with time. The results are mixed as clients have varied interests. It has been my experience that as models get more complicated, they are less likely to be used to make decisions. Simplicity and transparency are often critical to keep the discussion focused and to ensure the model is relied upon for its intended purpose.

Revisiting Zimmerman et al. (1998) Twenty-Five Years Later: What Lessons Did We Learn?...From One of the Survivors – Marsh Lavenue and Katie Markovich, INTERA Incorporated

In 1991, Sandia National Laboratory convened a panel of the leading groundwater inverse-problem researchers to review work done on the WIPP-site groundwater model developed by INTERA and to assess ways to incorporate uncertainty into the results. At the end of the initial meeting, the panel, named the Geostatistics Expert Group (GXG), concluded that an ensemble of calibrated transmissivity fields was needed to represent the uncertainty of the travel time to the boundary of the WIPP Site. This capability was added by the INTERA team some months later and the results were presented to the GXG. As a means to benchmark the new INTERA inverse code, called GRASP-INV, the GXG initiated a series of test cases and invited inverse researchers around the world to participate. Over the next two years, four test problems were issued to seven research teams. The objective for each test problem was to calibrate an ensemble of transmissivity fields to a limited data set of head and transmissivity values sampled from the 'real' models. This important work was published by Zimmerman et al. (1998). This presentation will review the GXG test problems and the keys to superior inversion performance.

Making the Most of Nothing – Jeremy White, INTERA Incorporated

The data scarcity of subsurface environmental simulation is the source of so many of our problems. We often lament how little we actually "know" about the aspects of the natural systems we are studying and modeling. Aren't we living in the information age? Maybe we need to rethink what it is to "know" something about these complex systems. For example, the location of a high-capacity extraction well must indicate a relatively high transmissivity in and around that location in the subsurface. Or a farmer may "know" that a certain field has never produced more than a certain yield in a growing season. Or site personnel "know" that certain monitoring wells go dry during sampling. Are these bits of knowledge useful? The answer is, as always, "it depends" (on many factors), but in some settings, when taken collectively, and in combination with other more traditional state estimates, the answer is a definitive "yes, these bits are valuable to reduce predictive uncertainty". A few recent experiences with trying to use these imprecise data will be presented.

Embracing the New School: a Successful Case Study Using PEST++-IES to Estimate Mine Dewatering Inflow – Gustavo Meza-Cuadra and Douglas Oliver, FloSolutions USA Ltd.

Traditional groundwater modeling workflows often culminated in a sensitivity/uncertainty analysis attempting to assess model output-to-parameter variation. This type of analysis, often referred to as "sensitivity" assessment, provided modelers a measure of parameter uncertainty in their output estimates, e.g., drawdown to hydraulic conductivity uncertainty. However, this assessment often was incomplete and lacking in thoroughness. With modern inversion methods applying Bayesian paradigms to model history matching this type of analysis has been superseded and translating parameter uncertainty into forecast models has become more mathematically rigorous, and just as importantly, straightforward to implement. The authors are frequently tasked with estimating groundwater inflow into mining operations. Mining methods generally involve extracting geological material and creating voids. To ensure safe mining operations, these voids need dry working conditions, i.e., mine dewatering. Groundwater modeling is the industry standard for estimating dewatering flowrates in these types of problems.

An underground mining operation required estimation of dewatering inflows for engineering considerations. Initially, a deterministic groundwater flow model was constructed. The model was calibrated using a combination of manual and inverse methods to a single best set of parameters. Using these calibrated parameters, a conventional sensitivity analysis was performed by constructing a series of predictive

simulations (mining) and a range of potential dewatering flowrates were estimated/s, with the high and low values based on specific hydraulic parameter value variations. While this type of workflow has been the industry standard for the past several decades (especially outside of academia), a new paradigm of quantifying uncertainty has developed and matured. Given the important decisions that are made during the engineering design process prior to mine development, understanding the risks and quantifying uncertainty in groundwater flow dynamics, a more rigorous approach is warranted. This is particularly true in heterogeneous and anisotropic hydrogeologic settings commonly found at mine sites, where spatial variations in the hydraulic property fields are important for future predictions. Previous generation modeling tools often provided a single best estimate of parameters (deterministic), and despite the limitations being apparent to most groundwater practitioners, computational constraints often made it impractical to generate multiple realizations of calibrated parameters. PEST++-IES (Iterative Ensemble Smoother), using novel mathematical methods, decoupled parameter estimation from computational burden using ensemble methods, and allows for multiple parameter realizations (ensembles) to be easily computed to better assess uncertainty. Using PEST++-IES, FloSolutions undertook an ensemble-based recalibration and uncertainty analysis for the proposed underground mine. An ensemble of 160 calibrated parameter fields were generated and used to run the forecast (mining) model. A range of flowrates was estimated with these realizations, and the median value was shown to be ~3x times higher than the value estimated with the deterministic model as previously assessed. Due to the large number of realizations, the P-10 and P-90 values were estimable. Comparative analysis of the two approaches indicate that the traditional scenario-modeling methodology applied was underestimating the uncertainty in predicted dewatering flowrates. The updated analysis allowed the mining company to better understand their water-related risks and improve their engineering designs.

Evaluating Recharge Estimation Scenarios and Its Implications on Groundwater Management – Ryan Harmon, INTERA Incorporated

In 1996, the Texas Legislature passed the Edwards Aquifer Authority Act, which created the Edwards Aquifer Authority (EAA) to regulate pumping from the aquifer and pursue a program to ensure that the continuous minimum springflows are maintained to protect endangered and threatened species to the extent required by federal law. The Texas Legislature amended the EAA Act in 2007 to form the Edwards Aquifer Recovery Implementation Program (EARIP) and directed the EARIP to work with the U.S. Fish and Wildlife Service (USFWS) to prepare the Edwards Aquifer Recovery Implementation Program Habitat Conservation Plan (EAHCP or Plan). The first EACHP (completed in 2013) is set to expire on March 31, 2028. In preparation for the next EACHP, we implemented a risk-based workflow to project future springflow outcomes under a range of possible future climate and water-use conditions.

Forecasts of future springflow patterns were developed probabilistically using the existing EAA surface and groundwater models, climate analyses, and pumping and permit data to represent possible future springflow patterns, as well as to estimate uncertainty in the minimum springflow proposed in the new EAHCP. PESTPP-IES (White 2018; White et al. 2020) [1] was used to re-train the watershed model Hydrologic Simulation Program in FORTRAN (HSPF). The PESTPP-IES derived ensemble of HSPF models, described the inherent uncertainty in the physical watershed representation embodied within HSPF, and thus were used with the climate scenarios to account for uncertainty in the transformation from future precipitation and temperature to future estimated recharge.

Future estimated recharge ensembles and water-use scenario ensembles were combined into a joint ensemble. This joint ensemble was propagated through the MODFLOW model to estimate an ensemble of possible future springflow outcomes. These springflow outcomes will be used to evaluate the performance of the EAA stage restrictions and EAHCP springflow protection measures under varying future forcing conditions,

including the effects of climate change. We expect the outcome from this advanced analysis will provide substantial risk-based guidance to inform the EAHCP renewal process.

White, J.T. 2018. A model-independent iterative ensemble smoother for history matching and uncertainty quantification in very high dimensions. Environmental Modeling and Software; and White, J.T., Hunt, R.J., Fienen, M.N., and Doherty, J.E., 2020,

Approaches to Highly Parameterized Inversion: PEST++ Version 5, a Software Suite for Parameter Estimation, Uncertainty Analysis, Management Optimization and Sensitivity Analysis: U.S. Geological Survey Techniques and Methods 7C26, 52 p., https://doi.org/10.3133/tm7C26.

Subjective Nature of the Prior and Some Repercussions of This – Catherine Moore, GNS

Currently Unavailable

New Regulations and Compressed Timelines: Combining Imperfect Data, Approximate Models and Uncertainty Analysis to Achieve Forward Progress – Robert Gailey, PG, CHG, R.M. Gailey Consulting Hydrogeologist PC

Environmental and resource management professionals working in California during the last 20 years experienced the rollout of many new regulations focused on protecting both the quantity and quality of groundwater. Implementation challenges included limited data and only rudimentary understanding of groundwater systems within the context of questions posed by the new regulations. Timelines for compliance were short, uncertainty abounded, and stress was high. In some cases, combining available data with relatively simple simulators and applying readily-implemented uncertainty analysis provided enough information for progress to be made. Two examples are provided to illustrate: 1) developing water quality monitoring program parameters for hydraulic fracturing operations (directly informed by analysis with PEST) and 2) evaluating groundwater management plans regarding potential impacts to domestic wells (inspired by PEST).

Water Quality Monitoring Parameters

As of January 2014, new regulation in California required that groundwater quality monitoring be performed by the oil and gas industry as a condition for permitting well stimulation treatment (including hydraulic fracturing) operations. The depths to which monitoring would occur were determined from site conditions. In many cases, monitoring requirements hinged upon the concentrations of naturally-occurring total dissolved solids (TDS) in the oilfield. In general, groundwater that contained less than 10,000 milligrams per liter (mg/l) TDS was to be monitored for constituents related to oilfield operations.

Applying the TDS evaluation criterion to determine how deep to monitor groundwater quality was hampered by a lack of information regarding the concentration distribution with depth. Groundwater containing 10,000 mg/l TDS was generally located at depths greater than those explored for water supply (fresh water defined as ,â§ 3,000 mg/l TDS). While petroleum exploration extended to much greater depths, the shallower and intermediate-depth strata were usually not sampled. However, geophysical logging was conducted at intermediate depths fairly frequently. As a result, there was interest in using geophysical logging data to estimate TDS concentrations for use in evaluating groundwater quality monitoring requirements in oilfields where well stimulation treatment operations occurred.

At a large California oilfield, field sampling and quantitative techniques were used to develop a model that estimated TDS depth profiles from apparent resistivity logs. Field sampling involved geophysical logging as well as collecting and analyzing formation water samples along a 1,600-foot-deep borehole. Quantitative techniques included 1) mathematically filtering out the residual effects of drilling mud on TDS measurements made on the formation samples, 2) calibrating with PEST the parameters for a model based on the Archie equation using results from the formation sampling along with apparent resistivity and gamma ray logs, and 3) performing model prediction uncertainty analysis with PEST (Likelihood Ratio Method). The result was a well-constrained predictor of TDS concentration based on observed resistivity from e-logs. By quantitatively establishing that uncertainty in the Archie model predictions was fairly low, a useful tool for evaluating

groundwater monitoring requirements relative to the new regulations was provided and permitting under the new regulations could proceed.

Domestic Well Impacts

As of January 2015, new regulation in California required that measures be taken to achieve sustainable groundwater management. After local agencies prepare management plans, 20 years are allowed to achieve sustainability using measures that generally include pumping reduction and recharge enhancement. The local agencies specify groundwater level management targets that are not expected to cause undesirable results (impacts) that are significant and unreasonable. Details of the management plans are reviewed by the State and public with the possibility of changes being required by the State.

Equitable sharing of the groundwater resource is a significant focus of management plan review with potential impacts to economically-disadvantaged communities, including domestic well owners, being quite important. Because there are many domestic wells in California (well logs exist for approximately 326,000 wells), it became clear early in the response to the new regulations that evaluating the sufficiency of groundwater management plans with regard to effects on domestic wells would require detailed analysis. However, very little data was available to inform the necessary work.

In response to the new regulation, the State made available previously-confidential data on well locations and constructions. A well impact and mitigation requirements model was created by combining the well inventory data with general principles for well operation and approximate costs for different types of well service. Model calibration was performed for a county in the San Joaquin Valley (Tulare) where 1) failure of domestic well supplies was tracked during the 2012 to 2016 drought and 2) seasonal water variations to groundwater depth were tracked annually. Because the model output integer results (a well is either impacted or it is not), a gradient-based optimization approach could not be used. Taking inspiration from previous work with PEST and making use of the good fortune that there were only two model parameter values to be estimated (age of well retirement and initial depth of pump), calibration was performed by an enumerated search of parameter space. Spatial correlation in the calibration residuals was used to calculate a square residual weighting matrix and improve the calibration. The Likelihood Ratio Method was used to quantify uncertainty, which was fairly low, and create a well-constrained predictor of well impact and mitigation requirements in response to declining groundwater levels.

Results for the limited geographic region initially considered were extended to a larger area of the San Joaquin Valley to evaluate potential impacts to domestic wells stemming from the details of groundwater management planning for the area.   Model prediction uncertainty was shown to scale with the magnitude of groundwater level decline by a factor of two to three within the range of conditions indicated by the management plans. This was considered reasonable for a screening-level analysis of the groundwater management plans. The analysis indicated a significant amount of impact, and it was clear that mitigation measures should be proactively implemented or details of the plans changed. Modifications to the management plans are currently under preparation. A summary of outcomes should be available by the conference.

(INVITED) Uncertainty Quantification for Subsurface Petroleum Reservoirs – Dean Oliver, NORCE Research

In this talk, I will describe the main principals of the ensemble Kalman-like data assimilation systems for parameter estimation — the basis of the approach as an approximation of a "minimization-for-simulation" method and a few algorithmic choices that make the method successful on large history matching problems. I illustrate the use of use of the methodology with a modest sized benchmark reservoir history matching case, where the ensemble Kalman-like methods outperformed all other approaches. I will additionally show how the posterior ensemble of realizations was used to optimise the expected behavior of the reservoir.

Despite the success, the ensemble methods have several limitations. The most severe might be the use of a single ensemble-average estimate of the sensitivity of observations to model parameters, which results in a uni-modal estimate of the posterior distribution for model parameters. The second major limitation might be the use of a minimization approach to posterior sampling without weighting of the realizations. I will discuss modifications to the algorithm that allow the use of local estimates of sensitivity for composite observation operators, and a second modification that allows computation of particle weights after assimilation of data.

Improving BeoPEST Performance – Willem Schreuder, Principia Mathematica

Doing things in parallel is easy. Doing things efficiently in parallel is hard. The talk explores reasons why when using N cores to run a BeoPEST job in parallel, the task does not complete in 1/N time.

The answer depends on numerous factors such as staging of input and output files, CPU, memory, cache and bus congestions, differences in run time, differences in network performance, CPU performance and master node performance, to name just a few.

The answer is very problem specific and there is not a single answer to what works best, but we explore some experiments you perform to find good solutions.

Make it Rain: An HTCondor Workflow for Uncertainty Analysis in the Cloud - Mike Fienen, USGS UMID WSC

Uncertainty analysis is important for decision making. The tools continue to mature in a robust, open-source environment. But at the same time, models continue to grow in complexity and forecast needs require sophisticated models with complex boundary conditions and linkages to other models. The result is a great computational burden to keep up with the "best practices" we know are important but are difficult to perform routinely.

At the 1 st PEST conference, it was suggested that the cloud should, in theory, bring practically infinite computing power to any user but the adoption has not met the initial promise, in part because on the cloud "the meter is always running." The inevitable dark alleys and flat tires inherent to environmental modeling become especially problematic when navigating a model through the uncertainty analysis underworld. These issues can be intimidating to users not accustomed to paying for every compute cycle they use, but is this actually different from the seemingly free cost of maintaining a cluster of physical machines? The costs of computing continue to drop in the cloud relative to the human cost of machine maintenance, hardware costs, power, cooling, and other costs to maintain on-premises resources. Moreover, the technical burden of understanding and implementing the networking and security protocols for a compute cluster to function correctly are important costs often not accounted for. The wide variety of environmental models needed for decision support precludes a single approach to compute infrastructure, but particularly for practitioners without ready access to an existing large computing resource, we propose here that cloud resources may be an effective way to improve history matching and uncertainty analyses for most models.

In this work we present an open-source workflow, leveraging the Amazon Web Services environment, by which a user can flexibly start up a cluster of (effectively) unlimited size, collapse it back down, and efficiently stage data and perform parallel runs with the PEST suite of tools, facilitated by the HTCondor run management software. An important aspect of using cloud resources is the potential for a lower carbon footprint due to optimization on the vendor's part. We will present costs, demonstrate the technical configuration, and provide some lessons learned from running problems at scale in this environment.

Light Speed Sensitivities Using Adjoint States With MODFLOW 6 – Mohamed Hayek, INTERA Incorporated

Sensitivity analysis of the numerical model describing physical systems is recognized as an important step for obtaining an enhanced understanding of system performance. Direct approaches to sensitivity analysis include the parameter-perturbation method and the sensitivity-equation method. These methods are computationally efficient only when the effects of a few uncertain parameters on a large number of performance measures are being evaluated. Common hydrologic modeling problems often involve the contrasting case of a few performance measures with a large number of uncertain parameters. For such situations, the adjoint sensitivity approach offers an elegant and computationally efficient alternative to direct sensitivity calculation methods. A non-intrusive adjoint sensitivity capability for MODFLOW 6, designed as MF6-ADJ (ModFlow 6 - Adjoint) has been developed and tested. The MF6-ADJ code has been implemented using the MODFLOW API which allows other programs to control MODFLOW and interactively change variables without having to modify the MODFLOW 6 source code. The results from the MF6-ADJ code showed excellent agreement with those from the parameter perturbation approach. The present version of the code is restricted to regular grids. Further implementations are in progress.

A Python Toolkit for Interactive Plotting of PEST++ Ensemble Information – Ryan Conway and Evan Christianson, Barr Engineering

An open-source Python package has been developed for generating interactive visualizations to aid post-processing of information associated with ensemble methods in the PEST++ software suite. The increasing use of ensemble methods in data assimilation and uncertainty analysis makes traditional methods for understanding model inputs and outputs cumbersome. Interactive visualization is an effective and efficient way to understand the distribution of parameter values and model forecasts associated with an ensemble. These interactive visualizations can play an important role in quality assurance and provide insight to model behavior. Object methods in the package build on existing PEST-related packages such as pyEMU, visualization tools in Plotly, and Pandas data structures to help streamline model development and review workflows, improve troubleshooting, and enhance transparency.

Improving Stochastic Modelling Workflow Visualization, Interrogation, and Interaction - Brioch Hemmings, GNS

There is a growing appreciation that the use of numerical modelling to support decision-making benefits from, or even requires, model uncertainty quantification. Unfortunately, this can often involve complex modelling workflows and complicate the visualisation and interrogation of the numerical model outputs. Ultimately, this can separate those involved in the decision making process from the information provided by the modelling workflow. If the stakeholder in a modelling study does not understand the information provided by the process, or if that information is, through oversimplification, incomplete or inaccurate, their subsequent actions may be inaccurate, inappropriate, and poorly communicated. Consequently (and somewhat ironically), this understanding gap can mean that the efforts to improve the robustness of modelling studies, through the use for stochastic methodologies, can undermine the trust in the modelling outputs and the decisions that they inform.

Aims - We aim to develop tools that support user interrogation and interaction with stochastic modelling workflows. These tools must mesh with prediction specific modelling frameworks that quantify and express model uncertainty. They need to be able to convey diverse and complex results from a variety of models. They also need to be relatively easy to construct and must not require additional specific computational specialties for the end user.

Methods - We develop a variety of example tools for visualisation, interaction and interrogation of stochastic groundwater modelling workflow results, through combining open-source, python libraries and cloud-based

server solutions. These tools can be by run by users from their browsers, without any requirement for specialist software or computational expertise.

Results - We demonstrate examples of these interaction and visualisation tools that give the power to interrogate, visualise and explore complex stochastic workflows at various stages in a modelling study, to a range of end users (e.g. Groundwater emergence mapping in South Dunedin, Figure 1.). The examples provide a starting point for standardising and generalising (where possible) the roll-out of visualisation tools, often within complex workflows, to improve trust and uptake in the use of robust modelling methodologies in decision support.

(INVITED) Utilizing Structured Decision-Making to Integrate Data, Modeling, and Science Into Policy Formulation and Implementation – Alyssa Dausman, The Water Institute of the Gulf

Utilizing models to inform policy is the "ideal" many strive towards, but doing so in practice can be quite challenging. This challenge often stems from the need for time and money to be spent on the front-end and back-end of model development to properly engage decision-makers in the process. In addition, models often need to be paired with multiple types of science and data to truly inform policy. To be effective, teams of researchers need to be interdisciplinary and diverse, often integrating lawyers, planners, economists, social scientists, and policy researchers into the teams that are developing the models. Having good facilitation and trust is also critical for success. This talk will demonstrate how structured decision-making (SDM) can be successfully implemented and provide examples of integrating models into decision-making and policy development, including groundwater management and climate mitigation.

The Context

Every day, decision-makers face complex choices with far-reaching consequences for people, communities, natural resources, and the environment. These choices are even more challenging when there are multiple stakeholders involved or when there is uncertainty in what the outcomes of decisions might be. SDM is an objectives-oriented, transparent process that can support decision-makers by providing a framework for engaging stakeholders and incorporating defensible, science-based tools for evaluating the tradeoffs between choices (Keeny 1992).

What is Structured Decision-Making?

SDM involves the use of a broad set of tools drawing from the fields of decision analysis, operations research, economics, human dimensions, management science, behavioral psychology, and expert judgment. Through a structured and defined process, decision makers and stakeholders can deconstruct the heart of the problem, systematically identify "out of the box" and win-win solutions, address uncertainties that may be leading to indecision, and use robust tools for predicting outcomes. This process allows decision makers to identify the choices most likely to lead to positive outcomes for all concerns.

Steps in SDM: PrOACT

- Define the decision context or problem (what it is that the decision-maker and stakeholders are making choices about?). Do they have legal mandates or statutory restrictions?
- Define fundamental objectives (what are the core concerns that stakeholders want to improve and/or other important considerations such as environmental justice, economics, etc.,?)
- Identify alternatives (what are the choices or sets of choices to decide between?)
- Conduct consequence analysis (what will the impacts of the alternatives be to the fundamental objectives? This step includes the use of data or models – which can be simple or complex - to predict what these outcomes will be.)

- Evaluate and optimize tradeoffs (what are the benefits across different objectives and what choice or sets of choices result in the most desirable overall outcome? This step can also include quantitative analysis tools of different complexity.)
- Decide and take action. This step is still in the hands of the decision maker, but the consequences and tradeoffs are transparent and based on robust tools. This step often includes legal and policy research on integration and implementation.

PrOACT

1. Define the **PR**oblem
2. Define the **O**bjectives
3. Identify **A**lternatives
4. Conduct **C**onsequences Analysis
5. Evaluate and optimize **T**radeoffs

Adapted from Jean Fitts Cochran

Examples of implementation by The Water Institute

Louisiana Climate Initiatives Task Force
Long-term Strategic Water Sustainability Plan: Capital Area Ground Water Conservation Commission

Doing Less for More: Coupling Multi-Dimensional Scaling and K-means Clustering for Efficiently Sampling the Posterior, Demonstration in an Aquifer Setting with Categorical Facies – Prashanth Khambhammettu, PhD, PE, Arcadis Inc.

The Traveling Pilot Point Method (TRIPS) has been recently developed to parameterize the categorical inverse problem in aquifer settings with categorical facies. In this paper, we successfully use an iterative ensemble smoother (IES) in conjunction with the TRIPS method to generate posterior parameter ensembles for a synthetic aquifer with a categorical distribution consisting of high-permeability channels incised in a low-permeability matrix. For this synthetic problem, as the prior ensemble size was increased, the posterior ensemble began to increasingly resemble an ensemble generated using rejection sampling. Multi-dimensional scaling (MDS) projection was used to illustrate the dissimilarity of the prior and the posterior ensembles and to demonstrate the unbiasedness of the posterior ensembles. An interesting finding was that the proportion of valid posterior realizations within the prior ensemble decreased with increasing sizes of prior ensemble. The best match to rejection sampling was obtained from a posterior ensemble with 1622 realizations. However, the performance of IES was comparable to other subspace-based inversion methods. Using MDS and K-Means clustering, we demonstrate that it is possible to strategically select a smaller number of prior realizations such that the resulting posterior ensemble would still have the statistical properties of a much larger posterior ensemble. The lessons learned from the synthetic problem could be used to test the feasibility of

TRIPS/IES/model selection techniques to solve more complex categorical inverse problems that are representative of the real-world.

An Empirical Evaluation of Sequential and Batch Data Assimilation Approaches to Cope with Groundwater Model Error – Katherine Markovich, INTERA Incorporated

Groundwater model error, arising from the inevitable simplification and abstraction modelers must make of complex real-world system and processes, has been shown to produce biased predictions as a direct result of parameter compensation during data assimilation. The specter of error especially plagues groundwater decision support modeling, since the inverse methods underpinning calibration and uncertainty analysis favor a computationally efficient and numerically stable model, or in other words, a simpler model. This work explores sequential data assimilation (DA) as a potential coping mechanism for the error encountered by simpler models. Unlike traditional batch methods, sequential methods assimilate data in discrete time intervals or 'cycles', and simultaneously estimate model state along with model parameters to advance the model forward in time. We hypothesize that the estimable model states in sequential DA afford more flexible and appropriate receptacles for the noise introduced into observations from model error. Using a paired complex-simple model approach, we empirically evaluate the predictive outcomes of batch and sequential DA in two model error scenarios: first where error arises from coarser resolution in the simple model, and second where error arises from both coarser resolution and fixed pumping rates in the simple model. Overall, we find that both formulations perform well in both history matching and forecasting when employing a high-dimensional parameterization stance, that is, treating all properties and stresses as uncertain and adjustable during the inversion process. When uncertain parameters are removed from the inversion process, however, the data assimilation process is degraded in different ways for batch and sequential formulations. These results have implications for groundwater decision support modeling as they underscore the pitfalls of fixing parameters a priori, such as with pumping, and present a proof of concept for using adjustable model states to cope with model error in decision support modeling contexts.

Rethinking Prior Parameter Uncertainty from Groundwater Model Calibration Results: Minimizing Underestimation of Predictive Uncertainty – Tomas Opazo, Flinders University

The goal of groundwater modeling is to support scientifically-based management of hydrogeological systems. It does this by associating probabilities with future system conditions under different proposed management scenarios. Bayes equation makes it clear that this requires that a modeler express his/her impressions of potential hydraulic property heterogeneity. These impressions are encapsulated in a prior probability distribution, or simply "the prior". Depending on the information content (or lack of information) of a history-matching dataset, model predictions can inherit considerable uncertainty from this prior. When a model is calibrated through numerical inversion, it is not uncommon to obtain a calibrated parameter field that exhibits greater spatial variability than that which is expected from the prior. This requires a rethinking of the prior in order to preclude underestimation of the uncertainties of decision-critical predictions. We show how the traditional utility of the model calibration process can be extended to estimate values not just for parameters used by a model, but also to explore the values of parameters that characterize the prior probability distribution of system properties. We show, using synthetic and real-world cases, that this can reduce the risk of understating the uncertainties of important model predictions when subjecting these predictions to Bayesian uncertainty analysis.

Spatial Averaging Implied in Aquifer Test Interpretation: The Meaning of Estimated Hydraulic Properties – Neil Manewell, University of Queensland

Processing of aquifer test drawdowns to obtain estimates of transmissivity, and sometimes storativity, is an integral part of hydrogeological site investigations. Analysis of these data often relies on an assumption of hydraulic property uniformity. Aquifer properties are often estimated by fitting a Theis curve to measured drawdowns. Where an aquifer exhibits heterogeneity, quantities that are forthcoming from such analyses are assumed to represent spatially-averaged properties. However, the nature of the averaging process, and the area over which averaging takes place are unknown. In this study we derive spatial averaging functions that link inferred hydraulic properties to real-world hydraulic properties. These functions employ Fréchet integrals derived by previous investigators that link observation well drawdowns to aquifer properties under an assumption of mild aquifer heterogeneity. It is shown that these hydraulic property spatial averaging functions are complex, especially at times that immediately follow the commencement of pumping. Furthermore, they cross hydraulic property boundaries, so that estimates of storativity can be contaminated by heterogeneities in real-world transmissivity, and vice versa. Because of its greater averaging area at later times, estimates of transmissivity are generally more immune to the effects of local hydraulic property heterogeneity than are those of storativity. They are therefore more reflective of broadscale real- world hydraulic properties, particularly those that prevail in areas that are removed from the immediate vicinity of the pumping and observation wells.

Calibrating and Quantifying Uncertainty for Complex Flow and Transport: Chromium and RDX Regional Models at LANL - Lauren Foster, Neptune

Two unique contaminant plumes below Los Alamos National Laboratory (LANL) property are characterized using similar methods but different models. A plume of hexavalent chromium (Cr6+ or Cr, in this document) has been detected in excess of the 50 ppb New Mexico groundwater standard in the central portion of the regional aquifer; the highest measured concentration is approximately 1,200 ppb. Additionally, a plume of the organic compound hexahydro-1,3,5-trinitro-1,3,5-triazine (Royal Demolition Explosive [RDX]) with concentrations greater than the New Mexico tap water drinking standard of 9.66 ppb is present in the western portion of the regional aquifer near the mountain block; the highest measured concentration in the regional aquifer is approximately 26 ppb. Numerical modeling is used to improve understanding of the plumes and inform decision-making around remediation strategies.

The modeling approach integrates all available information to inform decision-makers and stakeholders with reliable assessment, prediction, and uncertainty quantification. The steps developed for the modeling leverage all lines of evidence available, including site data, CSM and expert knowledge, as well as other information (such as focused data-based studies or pre-existing models). This site information is combined into the numerical model, which includes boundary and initial conditions, discretization in space and time, and simplifying assumptions. These lines of evidence also inform distribution development to constrain input parameters to plausible ranges and quantify the likelihood of certain values. Models are then calibrated against site data ("targets") and validated with data and conceptual information that were not used as targets. Modeling is inherently an iterative process and analytical tools are used at every step to improve process representation, input parameterization, and assumptions.

Calibration is performed using a Bayesian approach and vetted through hands-on expert interaction with the model. Multiple top calibrations are identified using a combination of forward draws across parameter prior distributions, hand-tuning, and leveraging a Levenberg-Marquardt (LM) algorithm. The challenges of the calibration include high temporal and spatial resolution, high-dimensional parameter space (including spatially heterogeneous material properties), high-dimensional target data sets, and complex flow fields. A discrete set of top-performing calibrations are used to estimate model uncertainty. Each of these then initializes a Markov

Chain Monte Carlo (MCMC) sampler to quantify parameter uncertainty and produce posterior parameter distributions.

Both the RDX regional model (RRM) and Chromium regional model (CRM) show very close matches between simulated and observed targets at the site; including timeseries of concentrations, hydraulic gradients (both direction and magnitude) local to the plumes, static water levels, and drawdown responses at monitoring wells from pump tests. Combined, these targets ensure confidence that the site physics and hydraulics are well represented in the model.

The method presented here for calibrating complex numerical problems and estimating uncertainty is effective for both contaminant plumes at LANL, though each contains a unique decision context, dataset, CSM, and challenges.

(INVITED) Why Are We Here? Reflections and Murmurings from an Industry Perspective, Keith Brown, Rio Tinto – Keith Brown, Rio Tinto

Currently Unavailable

A Bayesian Statistical Perspective on Calibrating Physics-based Groundwater Models – Leslie Gains-Germain, Neptune

Classical calibration techniques are used in groundwater modeling to find solutions that match observed data. A classical calibration involves identifying a deterministic model with one set of input parameters that minimizes the error between observations (target data) and simulation. Often when a groundwater model is to be used to support decision-making, uncertainty quantification is desirable and demands a statistical decision perspective. Uncertainty quantification can be difficult, however, since groundwater problems are often ill-posed (modeling terminology) or undefined (statistical terminology) when the number of parameters or unknowns outnumber the available data. Here, we present a Bayesian approach to uncertainty quantification that provides constraints needed to solve sparse data problems in a statistically rigorous way. The approach employs informative priors for parameter-heavy unknowns (i.e., unknowns that necessitate many parameters for characterization, for example, a heterogeneous hydraulic conductivity field) based on a combination of information from the literature, laboratory studies and subject matter expertise. Less restrictive, continuous prior distributions are retained for parameters thought to heavily influence the process of interest (for example, contaminant transport). Utilizing a combination of discrete and continuous priors facilitates a successful fit of a Bayesian model for an otherwise ill-posed problem. The approach successfully characterizes uncertainty through a statistical model while imposing sufficient prior constraint to ensure physical accuracy and meaningful results.

Evaluation of the Probabilistic Capture Performance of Horizontal Reactive Treatment Well (HRX Well®) – Jack Wang, Arcadis

The Horizontal Reactive Treatment Well (HRX Well®) is a new in-situ remediation concept that has been demonstrated via ESTCP projects [1] and has been installed at several sites to focus on long-term contaminant mass flux/discharge reduction [2]. Before field installation of HRX Well® at a site, site-specific groundwater models are developed to provide a quantitative framework to ultimately support the final design of HRX Well® including well location/orientation, screen length, and treatment media length. The primary objective of the groundwater model is to evaluate whether the design has met the performance objectives such as desired hydraulic capture based on remediation goal. In this study, MODFLOW-USG code was selected for simulation of groundwater movement in the aquifer. MODALL [3] was used to quantify the hydraulic capture of HRX Well® based on volumetric-tracking method, which offers an improved approach by directly quantifying the fraction of flow in each model grid cell that either originated from a given source or flows to a specified sink (i.e., capture fraction).

The original groundwater model was developed and calibrated under steady state conditions. Parameter adjustments were manual during calibration and the spatial parameterization of horizontal hydraulic conductivity was based on zones of piecewise constancy. The geometry of these zones was delineated based on inferences of hydraulic conductivity estimated from slug test results. The components of the HRX Well® were represented as high hydraulic conductivity fields with remarkably small cell dimensions of several inches to achieve numerical accuracy near HRX Well®.

To perform the probabilistic evaluation of the capture performance of HRX Well®, the original model was recalibrated with PEST_HP using pilot points approach that allows representation of geological heterogeneity

at a finer scale than zone-based approach and automatic adjustment of model parameters through regularized inversion. CLN package was used to represent HRX Well® due to its advanced capabilities to simulate horizontal well features without having to refine the numerical grid around the horizontal well as is done in a "traditional" modeling approach. Once a suitable fit had been attained with the calibration dataset using PEST_HP, the PESTPP-IES ensemble smoother was used to obtain a suite of parameter fields (stochastic parameter fields) that maintain the model a calibrated state as well as the parameter field obtained from PEST_HP to explore post-calibration predictive uncertainty.

The stochastic parameters field obtained from PESTPP-IES that were hydrogeologically reasonable were then used in conjunction with MODALL to delineate the hydraulic capture area of the HRX Well®. The capture areas estimated for all parameter fields are combined into a single probability capture map where 0.0 denotes cells that were never being captured and 1.0 represents cells that were always being captured among all the realizations.

The probabilistic capture of the existing HRX Well® design was then evaluated and compared with targeted capture width required by the remediation goal. The results suggested that the revision of HRX Well® design would improve the hydraulic capture performance and provide greater certainty in meeting the performance objectives.

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Applied Uncertainty Analysis for a Reactive Fate and Transport Numerical Model in a Highly Controlled Remedial Injection – Melanie Beck, Parsons

Numerical models can be invaluable tools for decision making in remedial designs, where the effectiveness of the design rests upon evaluation of the site hydrogeology. In situ remedies can often prove more challenging due to the complex hydrogeologic and geochemical systems, resulting in potential inefficiencies in the treatment. For a site in northeastern United States a pilot test was developed and performed for in situ treatment of elevated arsenic concentrations and dissolved hydrocarbons associated with residual Light Non-Aqueous Phase Liquid (LNAPL) in glacial deposits within a small coastal stream valley. Historical chemical manufacturing operations resulted in an arsenic plume that, prior to pilot testing, was undergoing a typical groundwater pump and treat. A pilot was designed and implemented for sulfate injection to treat dissolved hydrocarbons and potentially treat the arsenic concentrations abiotically. A MODFLOW-USG groundwater flow and sulfate fate and transport model were developed, calibrated, and sensitivity tested to provide hydrogeologic support testing of in situ treatment with sulfate. The modeling included: (1) calibration to steady-state static and pumping conditions in order to refine parameters such as hydraulic conductivity, recharge, and boundary conditions, (2) sensitivity testing of hydraulic parameters using PEST, (3) simulation of groundwater flow patterns for pilot test support, (4) model field verification to pilot test data, (5) calibration to transient sulfate fate and transport data using PEST, (5) evaluation of hydraulic and transport parameter uncertainty using PESTPP-IES, and (6) optimization of sulfate injection using PESTPP-OPT. Results of the uncertainty and optimization analysis improved the design team's decision making via: improved hydrogeological detail including sensitivity of upland geological pinch-outs, optimization of risk versus effectiveness relative to injectate concentration and flow rates, and (3) spatial and temporal heterogeneity of sulfate decay. Results from PESTPP-IES analyses exposed spatial regions of greatest uncertainty in sulfate fate and transport, which provided the design team with areas of highest failure risk. Results from PESTPP-OPT

analyses provided the design team with optimal injection well spacing to achieve coverage of the target treatment area, as well as optimal design flow rates and injectate concentration given the remedial design constraints. This predictive and uncertainty modeling of a highly controlled / monitored long-term field injection was an effective tool for: evaluation of treatment transport, quantification of risk of design failures, as well as communication to clients and regulators. This project provides the numerical modeling community an example of how advances in modeling capabilities (particularity recent uncertainty applications) can improve modeling applications, as well as modeling acceptability by influential stakeholder (i.e. clients and regulators).

Combining Weather Forecast and Groundwater Modelling Ensembles to Quantify Predictive Uncertainty Under Climate Change – Johanna Zwinger, INTERA Incorporated

Predictive modelling includes assumptions about system variables in the future. In groundwater flow modelling often one of the main driving variables is the amount of rainfall. At the same time long-term weather forecasts and impact of climate change come along with high uncertainty. To overcome this problem, classic predictive modelling often uses a single "worst case" climate change scenario. This study presents a possibility on how weather forecast uncertainty can be included in predictive groundwater modelling. The aim of this approach is to propagate uncertainty from the weather forecast into groundwater predictive uncertainty analysis, by combining weather and groundwater parameter ensembles. Forty-eight different climate change scenarios, ranging from wet to dry scenarios, were available from the Department of Water for the study site in Western Australia. The upper and lower 90% interval and median were used to create an ensemble of normal distributed climate change scenarios between those bounds. Those scenarios were multiplied with local rainfall time series from monthly mean values of the model calibration period and randomly assigned to the predictive model ensemble. This led to predictions accounting for model parameter uncertainty and climate change uncertainty and provided more reliable model predictions.

Current and Future MODFLOW-6 Development – Chris Langevin, USGS

Currently Unavailable

The MODFLOW-6 API – Joe Hughes, USGS

Currently Unavailable

Stochastic, Flow Regime-Dependent Estimates of Stream Gauge Discharge Measurement Error for Hydrologic Model Uncertainty Analysis with Ensemble Methods – Nick Martin, Southwest Research Institute

Stream gauge discharge data are commonly used as calibration data for hydrologic and hydrodynamic models. Most stream gauge discharge data are derived or calculated from measurements of water depth or stage using a rating curve. Consequently, stage is typically the observed or measured value, and discharge is calculated or modeled using a transform function. Observation uncertainty for stream gauge discharge is comprised of both measurement and model error and ranges from ±20% of calculated discharge to more than ±100% of calculated discharge. Expected uncertainty in stream gauge discharge data is largest for low flows, smallest for medium flows, and is larger (relative to medium flows) for high flows. A stochastic, statistical method for estimating flow regime-dependent, stream gauge data uncertainty is presented. This method is designed, and was developed, to produce standard error estimates for each time interval in a transient calibration data set that can be used in ensemble approaches as a description of 'measurement noise'. Additionally, the method provides for estimation of goodness-of-fit measures, like Nash-Sutcliffe Efficiency (NSE) and Kling-Gupta Efficiency (KGE), between the calculated stream gauge calibration data set and estimates of the 'true' discharge data set.

Tuning a Remediation System on Long Island in the Face of Uncertainty: A Journey in Ensemble Methods and Constrained Optimization – Nicholas Corson-Dosch, Upper Midwest Water Science Center, USGS

Past practices at a former industrial-military facility on Long Island, New York led to the contamination of the local groundwater system with chlorinated solvents. Eleven public water supply wells have been affected by groundwater contamination originating from the facility and an additional 16 public water supply wells are now considered threatened. In 2019, a remedial strategy was developed to address the contamination concerns that targeted full hydraulic containment of the contaminant plume using a combination of pumping wells, injection wells, and infiltration basins. In support of this remedial strategy, we developed two MODFLOW 6 groundwater model ensembles, based on two conceptualizations of subsurface properties, and leveraged the PEST++ suite of tools to evaluate the effectiveness of the proposed remedial design and optimize its performance under uncertainty. We developed our model as an inset, extracted in a repeatable workflow approach from a regional "parent" model, focusing in on the area of concern with refined spatial discretization and streamflow routing. We performed history matching on both models using PESTPP-IES, resulting in posterior parameter ensembles that produced overlapping but distinct ranges of prediction uncertainty. We then used the posterior parameter ensembles in a particle-tracking and MODFLOW 6 Transport Monte-Carlo analysis to evaluate the range of simulated hydraulic containment using the initial remedial design pumping rates. We identified a suite of risk-averse, risk-neutral, and risk-tolerant posterior ensemble members from this analysis based on the distribution of predicted hydraulic containment across the ensembles. These ensemble members provided the seed for constrained optimization, evaluating the competing interests of sufficient extraction and treatment to remediate and prevent further migration of the plume, while constraining the remedy to not induce flooding when returning treated water to the aquifer. A systematic sweep across the risk profile and profile of plume capture and the remediation pumping rates prior to formal optimization using PESTPP-OPT was found to be extremely valuable to the process leading to an understanding of the tradeoffs among the competing factors. The optimization objectives involve maximizing the capture by remediation wells and minimizing capture by non-remedial water supply wells. This presentation will focus on preliminary findings and some of the lessons learned from our approach.

Using Management Optimization Under Uncertainty to Support Groundwater Management in Island Aquifers: An Application in the Magdalen Islands (Canada) – Cecile Coulon, INTERA Incorporated

In coastal zones and islands, seawater intrusion is a main threat to water supply systems, since the excessive pumping of fresh groundwater can lead to the salinization of production wells. These zones are also confronted by rising sea levels, modifications in groundwater recharge and increasing water demand. The implementation of management optimization under uncertainty is highly valuable, to identify optimal management solutions and to quantify the impact of uncertainties on optimal management strategies. However, the large simulation times associated with dispersive solute transport models (in which fresh and saline groundwater can mix) severely limit the implementation of pumping optimization under uncertainty in real-world, large-scale models. Both deterministic and ensemble-based frameworks were developed to optimize pumping rates in island aquifers considering parameter, observation and climate uncertainty, using a sharp-interface model (in which mixing between fresh and saline groundwater is neglected) and the PEST/PEST++ tools for data assimilation and management optimization under uncertainty. In the deterministic approach, data assimilation was conducted using PEST_HP and pumping rates were then optimized using PESTPP-OPT and linear uncertainty estimates. In the ensemble-based approach, data assimilation was conducted using PESTPP-IES and pumping rates were optimized using PESTPP-MOU and ensemble-based uncertainty estimates. Both frameworks considered parameter uncertainty, observation noise and projected recharge and sea-level rise uncertainty, and the optimization results were compared to projected water demand uncertainty. These frameworks enabled the quantification of the optimal tradeoff between pumping and risk of well salinization. A set of maximum acceptable pumping rates was obtained for a wide range of

risks, which allows groundwater managers to select their preferred management scenario depending on the level of risk that they consider to be acceptable. These methodologies were developed to address groundwater management challenges in a Canadian archipelago, the Magdalen Islands, and the deterministic framework was applied to the municipal water supply system of the archipelago's four main islands. Both frameworks were entirely scripted using Python and could be used to support decision-making in other coastal zones or islands.

Smoothed Frequency Map of Technetium-99 Concentration Plumes Used as Target for Calibration of Fate and Transport Model – Trevor Budge, INTERA Incorporated

Post-audit of numerical fate and transport model simulation results indicated the need to update calibration of hydraulic properties near an observed technetium-99 contaminant plume at the Hanford Site, Washington, USA. The technetium-99 contaminant plume is located in a region of the Hanford Site that is characterized by an extremely flat hydraulic gradient (~4e-6 m/m) to the point that measuring the flow direction is difficult [1]. Previous model calibration had relied on hydraulic head and gradient observations for quantitative targets and the historic tritium plume extent as a qualitative calibration target. Given the difficulty of measuring the hydraulic gradients in this region of the site, historic plume maps of technetium-99, created annually over 24 years (1995 to 2018), were utilized to provide observation data regarding flow direction. The data were used to create a smoothed frequency map to provide a set of quantitative targets to include in the calibration process that constrains the assignment of hydraulic properties. The smoothed frequency map was created by: 1) compiling the annual plume maps, 2) categorizing each cell in the numerical model as either within or without the contaminant plume based on the maximum contaminant level of 900 pCi/L for each year, 3) summing the number of times each cell was within the plume boundary and dividing by the total number of years, and 4) performing an inverse distance weighted interpolation of these values to smooth sharp differences between values in neighboring cells. The smoothed frequency map was developed to reduce discontinuity in the historic plume extents where the process of plume estimation has been completed through hand drawn contours, interpolation techniques, and a combination of the two methods at different points in the 24-year window. Calibration targets were utilized as a part of a systematic calibration using PEST and PEST_HP to minimize the objective function regarding the technetium-99 targets while maintaining the calibration to the hydraulic head and gradient targets. Overall, the objective function related to the plumes dropped roughly 50% over the pre-calibration value and the portion attributed to the heads remained relatively the same as the previous model.

1. U.S. Department of Energy, Hanford Site Groundwater Monitoring Report for 2020, Richland Operations Office, Richland, Washington, 2021; DOE/RL-2020-60, Revision 0.

Closed-Loop Decision-Support Modelling – Rui Hugman, INTERA Incorporated

Groundwater modelling is a valuable tool for informing future management actions, especially when the groundwater system is facing a new stress or condition for which there is no historical precedent. In such cases, the most valuable data to inform a decision is usually obtained after it is implemented. Traditional approaches to modelling rarely make the best use of this fact. Yet, advances in quantity and quality of data that characterizes various aspects of groundwater systems is growing rapidly, increasing the value of more frequent modelling-based data processing to support decision making.

We present a workflow for efficient, semi-autonomous higher frequency modelling in a decision-support context. Using closed-loop management, we demonstrate how data assimilation and management optimization under uncertainty can be used to not only extend the lifespan of groundwater resources, but also to provide more frequent and accurate forecasts of future conditions. We apply this workflow to a synthetic coastal groundwater system facing overexploitation, reduced rainfall, and rising sea levels, with the goal of

maximizing the longevity of freshwater pumping. To measure the value of higher frequency updating, we repeat the workflow for multiple realizations of the truth.

Optimisation of Prediction-Driven Field Investigation Programmes Using Data Space Inversion and PESTPP-MOU – Eduardo DeSousa, INTERA Incorporated

Contemporary techniques in Data Assimilation, Uncertainty Quantification and Sensitivity Analysis allow the assessment of predictive uncertainty (and the ability of data to constrain it) at relatively low costs, especially when compared to costs associated with field investigations. In these contexts, the use of Data Worth Analysis before the implementation of field programmes can be extremely valuable in not only informing, but also establishing trade-offs between field investigation expenditure and reduction in predictive uncertainty. A case study is here presented for a site in southeast Asia, where a extremely costly drilling programme has been proposed in order to characterise the hydrogeological and geothermal regimes. A combination of Data Worth Analysis utilising an Ensemble Data Space Inversion and PESTPP-MOU has been applied to identify optimal well configurations for different number of wells, as well as the pareto fronts considering investigation costs and reduction in predictive uncertainty. The results show that with approximately 2/3 of the initial number of wells (22), 90% of the uncertainty reductions that would be achieved by the entire drilling program was obtained, resulting in significant cost and logistical savings for the project.

(INVITED) Decision-Support Modelling: Decomposing the Problem and Why it Matters – John Doherty, Watermark Numerical Computing

Why do we model to support decisions? More often than not, it is because we are scared not to model. Why do we make models so complex? More often than not, it is because we fear harsh judgment delivered by those whose reputations are buoyed by the eloquence of their criticism of us.

Too often, groundwater modelling is a primeval ceremony that is mandated to precede the making of expensive decisions. The gods of partial differential equations are invoked in order to provide us with digital fantasies of the subsurface. While this intricate numerical ritual can protect decision-makers from their political enemies, its connection with the scientific method is often tenuous.

So what does more scientific-based decision-making look like? Information (by definition) reduces uncertainty. It follows that scienced-based decision-support modelling should be designed to harvest information from data. It should also quantify the implications of information insufficiency; decision-makers need to know whether bad things can accompany certain courses of management action before they actually embark on them. Fortunately, we have the numerical tools to do all of these things.

However, scientifically-based decision-making delivers more than this. The scientific method provides an unbroken chain of logic that can inform all aspects of model design. These include whether we need to model at all, whether we need one model or many, whether these models should be simple or complex, transient or steady state, single or multi-layered. Science can also assist us to implement history-matching in ways that reduce predictive bias, while ensuring that the uncertainties of decision-critical model predictions are reduced as much as information allows, while not being under-stated.

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