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Providing guidance for remediation planning through probabilistic modelling and multiple conceptual models

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Abstract

Effective mine and tailings remediation planning is critical to minimise long-term environmental risks. Predictive decision-support modelling can improve remediation planning and risk-based decision-making by quantifying the uncertainty of model predictions of interest and identifying reliable remediation strategies in the face of uncertainty. Uncertainty, and therefore reliability and risk, must be treated conservatively. Predictive uncertainty analysis typically focuses on quantifying and representing uncertainty in model inputs such as hydraulic properties and climate forcings, with the implicit assumption that the underlying model structure and conceptualisation are known. Although non-uniqueness in the conceptual model can strongly affect model predictions, accounting for conceptual uncertainty remains a challenge.

A decision-support tool was developed to estimate the probability of exceedance of groundwater standards by constituents of concern at a compliance boundary for multiple conceptual site models (CSMs). Each CSM could exert important controls on plume migration as well as the performance of remediation measures. The tool consists of an automated, rapid, and fully-scripted workflow which performs the following actions with little or no practitioner intervention for each plausible CSM: (1) construct a detailed site-specific groundwater flow and transport model, (2) conduct high-dimensional nonlinear history matching using an iterative ensemble smoother, (3) implement a range of possible remediation system configurations comprising source removal, a pump-and-treat system, and permeable reactive barriers, and (4) carry out a multi-objective optimisation analysis using the non-dominated sorting genetic algorithm NSGA-II to explore trade-offs between economic and environmental considerations as well as reliability.

The use of an automated modelling workflow enabled the evaluation of predictive uncertainty across multiple CSMs for a large number of remediation strategies, and the identification of reliable remediation strategies considering uncertainty. The approach was implemented using freely available, open-source modelling tools and is readily adaptable to other remediation planning contexts.

Keywords: *groundwater, remediation, conceptual uncertainty, optimisation under uncertainty*

1 Introduction

Uncertainty quantification is an important component of remediation planning, since a remediation system which is designed without accounting for uncertainty might fail to achieve its objectives when considering the uncertainty inherent in the understanding of many mining hydrogeological systems. On the other hand, explicitly accounting for model predictive uncertainty enables the identification of more reliable remediation strategies. These are strategies with a high probability of satisfying regulatory, environmental and technical constraints or which, to put it another way, have a low probability of failure, despite the recognised sources

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of uncertainty. While reliability can be also achieved through over-design – for example, by using an engineering safety margin – this approach leverages modelling and data to achieve reliability while avoiding unnecessary over-design and associated costs.

In groundwater science, model predictive uncertainty stems primarily from information deficits and can be categorised into many distinct types, including conceptual, parameter and observational uncertainty. Formal data assimilation techniques recognise and account for several sources of uncertainty including parameter uncertainty and measurement noise. Ultimately, they aim to robustly assimilate information towards making optimal predictions while providing estimates of uncertainty in these predictions.

The standard practice in applied groundwater modelling consists of developing a single conceptual site model (CSM) based on all available data and system knowledge, and treating this conceptualisation as fully known throughout the modelling process. However, given the limited amount of data and the simplifications required in representing complex subsurface systems, there may be a high degree of conceptual uncertainty in the CSM. Dealing with conceptual uncertainty is a challenge and it is often omitted from uncertainty analyses, which can lead to an overestimated reliability of the remediation design (e.g. Chitsazan et al. 2015).

Multimodel approaches can address conceptual uncertainty by developing, testing and using alternative CSMs to evaluate predictive uncertainty (Enemark et al. 2019). This study presents an application of a multimodel approach to investigate remediation measures at an undisclosed site. At the site, seepage from tailings impoundments has entered groundwater, elevating the concentration of constituents of concern (CoC). A multimodel approach was adopted to account for the possibility that various complexities may be controlling groundwater flow and solute transport processes at the site. A workflow was developed to: (1) estimate the probability of exceedance of groundwater standards by CoCs at a compliance boundary across multiple CSMs, and (2) to evaluate the potential reliability of alternative remediation strategies considering conceptual, parametric and observational uncertainty.

2 Methods

The workflow is summarised in Figure 1 and explained in the following sections. It uses widely available, open-source modelling tools and is entirely scripted using Python to automate the model development, data assimilation and uncertainty analysis of each CSM.

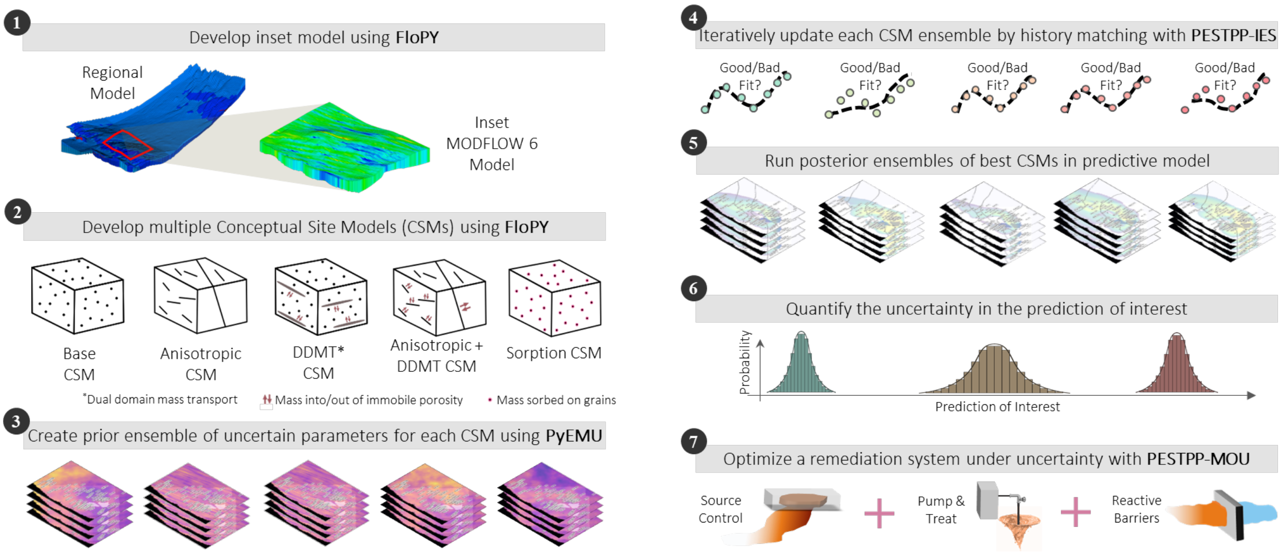


Figure 1 Workflow steps for the multi-model approach. DDMT = dual domain mass transport; CSM = conceptual site model

2.1 Development of multiple conceptual models

An inset MODFLOW 6 model (Langevin et al. 2017) is first developed from a pre-existing regional-scale groundwater model around the area of interest using Python scripting and the FloPy library (Bakker et al. 2016). Within this inset model structure, 5 groundwater flow and transport CSMs are developed, each representing a plausible CSM that could be important to the prediction of interest. All CSMs simulate flow, advective transport and hydrodynamic dispersion using heterogeneous hydraulic and transport properties. Each CSM explores an alternative conceptualisation that could exert important controls on plume migration and impact the simulated performance of remediation technologies. These are:

- Base CSM: spatially isotropic hydraulic properties
- Anisotropic CSM: spatially anisotropic hydraulic properties that represent possible preferential flow pathways related to geological structures at the site
- Dual porosity (or dual domain mass transport, DDMT) CSM: spatially isotropic hydraulic properties and dual domain porosity mass transport, where the dual domain porosity represents a possible mechanism for the CoC to have diffused into less mobile hydrogeologic units (e.g. fine-grained units) during historic loading, only to back-diffuse during active remediation
- Anisotropic dual porosity (or DDMT) CSM: spatially anisotropic hydraulic properties and dual domain porosity mass transport, where the dual domains comprise a small volume fraction of highly mobile fracture pathways and a large volume fraction of moderately mobile unfractured porous medium pathways
- Sorption CSM: spatially isotropic hydraulic properties and sorption processes, where CoC transport is retarded by sorption.

All CSMs use the same high-dimensional parameterisation scheme that attempts to represent expected spatial heterogeneity in both hydraulic and transport properties as well as uncertainty in historic flow and transport boundary conditions. In short, all model properties and model stresses are considered uncertain and therefore adjustable. Nearly 100,000 adjustable parameters are defined for the base CSM, reflecting spatial and temporal heterogeneity and uncertainty at various scales that are considered potentially relevant to the simulation of remedial actions. The CSMs that simulate additional transport processes introduce new parameters, which are also subject to high-dimensional parameterisation (e.g. the mass transfer coefficient for the DDMT CSMs, or the distribution coefficient for the sorption CSM).

2.2 History matching-based hypothesis testing

The 5 alternative CSMs are evaluated through history matching-based hypothesis testing. An observation dataset comprising approximately 2,000 transient groundwater levels and CoC concentrations is prepared and processed to be used for assimilation; these observations span periods of multiple decades, including initial loading, previous remedial efforts and a subsequent rebound in concentrations. Prior probability distributions functions (PDFs) are defined for all adjustable model parameters and parameter realisations are drawn from these prior PDFs to form a CSM-specific prior parameter ensemble. History matching is then conducted for each CSM using the iterative ensemble smoother implemented in PESTPP-IES (White 2018). The prior parameter ensemble is updated through history matching; generating a CSM-specific posterior parameter ensemble containing equally plausible parameter realisations honouring both expert knowledge and the observation data.

The underlying hypothesis being tested is that each CSM can produce a satisfactory fit to the observation dataset using reasonable parameter values. After history matching, a CSM can be rejected if the posterior ensemble yields an unsatisfactory fit to key aspects of the observation dataset, or if it yields a satisfactory fit at the cost of unrealistic posterior parameter values, where expert knowledge is used to define ‘unrealistic’ (Dausman et al. 2010). The CSMs that cannot be rejected are carried forwards for the remainder of the remedial action simulation analysis. For each remaining CSM, the posterior parameter ensemble is used to evaluate the probability of exceedance of groundwater standards by CoCs at the compliance boundary.

In the predictive period of the simulation, remediation technologies comprising source removal, pump-and-treat systems with water reinjection, and permeable reactive barriers are simulated to evaluate their combined ability to remove dissolved-phase CoCs. The MODFLOW Application Programming Interface (API) is used to simulate the reactive barriers and the pump-and-treat system (Hughes et al. 2022). For each retained CSM, the probability of CoC exceedance of groundwater standards at the compliance boundary is evaluated for multiple configurations (e.g. varying number and location of wells or barriers) and combinations of remediation technologies.

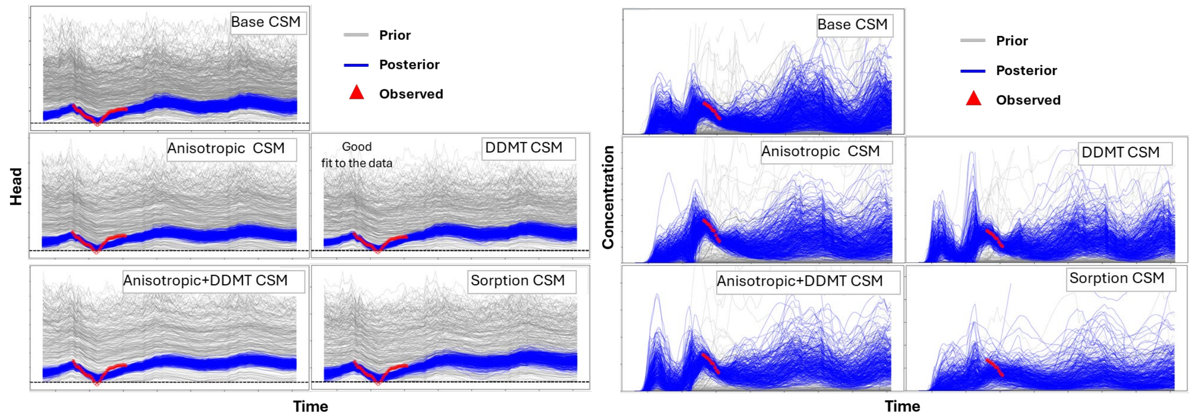
2.3 Remediation optimisation under uncertainty

A preliminary multi-objective management optimisation analysis is implemented in the workflow for a selected remediation system and a selected CSM. A remediation system is designed in which over 30 options for extraction-injection wells pairs are allowed to be put into operation at the start of the predictive period, source removal occurs, and several reactive barriers are allowed to be put into operation after 25 years of active pump-and-treat operations. Several optimisation formulations are tested to explore the trade-offs between economic and environmental considerations and reliability. All optimisations are subject to a strict constraint that the simulated concentration of CoCs must remain below groundwater standards at the compliance boundary. This constraint enforces containment of the CoC plume within the site and prevents the spread of CoCs beyond the boundary. The decision variables comprise extraction rates, duration of the pump-and-treat system, and barrier mass removal efficiencies. The use of multiple wells pair options is intended to offer flexibility during the optimisation rather than to suggest that all technologies must be deployed at once.

An initial optimisation formulation is explored which maximises mass removal while minimising water extraction. Maximising mass removal aims not only at containing the plume but also at actively reducing CoC concentrations within the site, whereas minimising water extraction aims at reducing both capital and operational costs. Other formulations are explored, which minimise either water removal or the duration of the pump-and-treat system (i.e. to minimise costs) while attempting to maximise reliability. The multi-objective optimisation under uncertainty problem is solved using particle swarm optimisation (Kennedy & Eberhart 1995) within the multi-objective NSGA-II evolutionary algorithm (Deb et al. 2002) and reliability-based optimisation (Deb et al. 2009) implemented in PESTPP-MOU, a tool for constrained single- and multiple-objective optimisation under uncertainty (White et al. 2022).

3 Results

Running the workflow up through the predictive uncertainty analysis (steps 1-6 in Figure 1) for all 5 CSMs requires less than 30 hours and needs no practitioner intervention. This is enabled by using a scripted approach that automates CSM construction, parameterisation and history matching, and high-performance computing resources. All CSMs show a reasonable fit to observed groundwater levels (Figure 2a) and CoC concentrations (Figure 2b). Furthermore, the posterior ensembles are narrower than the prior ensembles, indicating a reduction in model predictive uncertainty for all CSMs through history matching. The posterior parameter ensembles from all CSMs yield plausible values and patterns with respect to expert knowledge. Since all CSMs show a reasonable fit to data and have plausible parameters, none can be excluded and they are therefore all carried forwards into the predictive analyses. Some approaches have been suggested in the multimodelling literature for identifying data likely to discriminate between models (e.g. Wohling et al. 2015). In an effort to reduce the number of plausible CSM, additional targeted field data are currently being acquired.

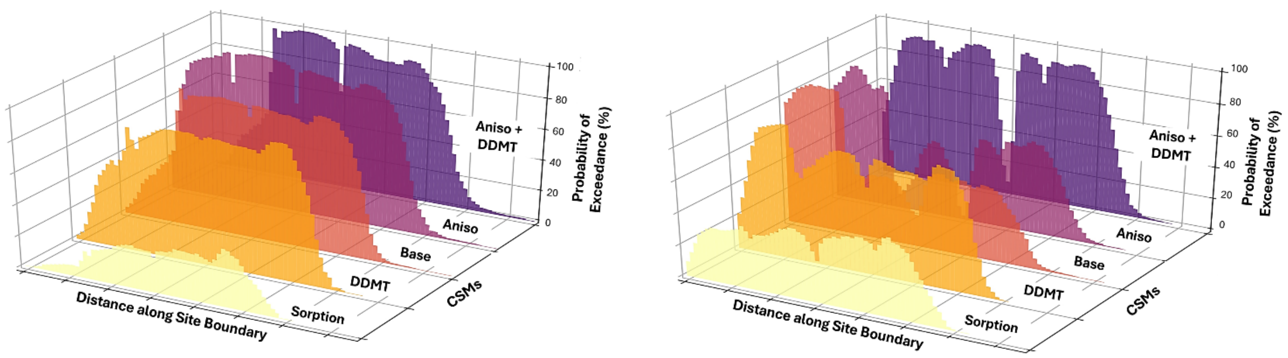


(a) (b)

Figure 2 Simulated versus observed. (a) Groundwater levels; (b) Constituents of concern concentrations at a monitoring well. DDMT = dual domain mass transport; CSM = conceptual site model

Without remediation, the probability of exceedance of groundwater standards by CoCs at the compliance boundary is above zero for all CSMs, indicating a near certainty of non-compliance with no remedial action. The sorption CSM shows the lowest probability of exceedance, whereas the anisotropic DDMT CSM shows the highest probability of exceedance. This pattern can also be observed in Figure 3, which shows the probability of exceedance of groundwater standards with a possible remediation configuration. Although the sorption CSM has the lowest probability of exceedance within a 100-year period, it would likely result in the most persistent exceedances over longer timescales (i.e. decades or more).

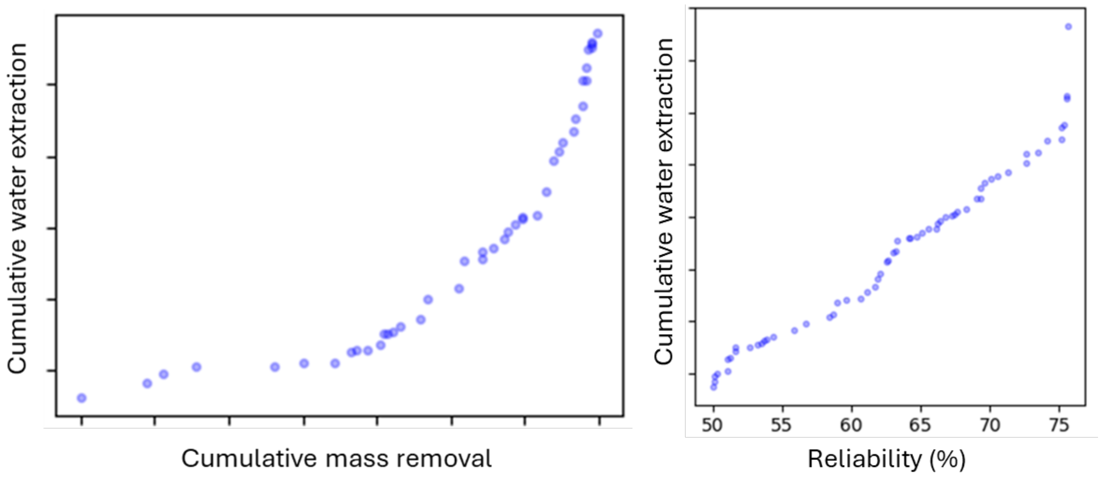
Comparing the probabilities of exceedance across multiple CSMs provides insight into how the performance of remediation strategies varies as a function of the CSM assumptions. While alternative approaches such as Bayesian model selection or averaging could be explored (Höge et al. 2019), comparing the results of predictive uncertainty analysis across all CSMs provides valuable insight into how predictions of management interest vary depending on the CSM. For example, in the anisotropic dual porosity CSM, the large amount of mass retained in immobile porosity limits the mass removal efficiency of the pump-and-treat system, which directly affects the desire to limit the duration of active remediation (Figure 3).



(a) (b)

Figure 3 Probability of exceedance in (a) 25 years and (b) 100 years with a possible remediation configuration

Through multi-objective optimisation, the optimal trade-off surface between conflicting objectives (also called a Pareto front) can be directly estimated. Figure 4a demonstrates the expected trade-off between cost (water extraction) and mass removal. As expected, costs increase with mass removal. Initially, large amounts of mass can be removed for relatively small increases in cost, but diminishing returns arise as further removal is associated with a substantial cost increase. Figure 4b demonstrates the expected relationship between cost (water extraction) and reliability. As more groundwater is extracted and treated, there is greater confidence that the concentration of CoCs will be satisfactory at the compliance boundary. However, the maximum achievable reliability for this specific optimisation is 75%. This implies that because of model input uncertainty, the combination of proposed remedial actions cannot provide 100% confidence that groundwater CoC concentrations will satisfy compliance. Uncertainty reduction through data acquisition or a redesign of the remediation strategy could increase this reliability. Rather than being caught off guard by failure, this approach facilitates the early identification of failure and provides the opportunity to prepare or hedge against it.



(a) (b)

Figure 4 Preliminary optimisation analysis of optimal trade-offs between (a) water extraction and mass removal and (b) water extraction and reliability

Both the remediation system used for the preliminary optimisations and the optimisation formulation are likely to evolve as the project progresses and new information is acquired to better align with site-specific conditions, management objectives and constraints. For instance, another remediation metric could be defined, such as unit of contamination removed by water managed. Mass removal, water extraction and reliability could all be simultaneously considered in the optimisation objectives. Water extraction is not the only expense associated with remediation and a cost objective function could explicitly account for various capital and operational costs (e.g. water extraction, water treatment). Furthermore, the multimodel approach could be incorporated into the optimisation design to find a remediation strategy that is cost-efficient and reliable across all CSMs (Elshall et al. 2020).

4 Conclusion

This study developed a multimodel decision-support tool to provide guidance for mine and tailings remediation planning. It enables decision-makers to evaluate the performance and reliability of different groundwater remediation strategies in the face of uncertainty. It also supports risk-based decision-making by quantifying the probability of exceedance of groundwater standards across multiple CSMs. The scripted approach allows modellers to easily and efficiently adjust model inputs and parameters, rapidly evaluate predictive uncertainty across multiple conceptual site models and explore different remediation optimisation formulations. This approach uses open-source tools and can readily be implemented to other contexts.

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