# Navigating groundwater model uncertainty analysis

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## Abstract

The design of a groundwater model is based on the model objective, the management or research question that the model seeks to address. Designing the uncertainty analysis of a groundwater models likewise needs to consider the objective of the uncertainty analysis; how the uncertainty in model predictions will be used.

In this paper a framework is presented to consider the various dimensions of groundwater modelling and uncertainty analysis. The discussion is structured around four main types of groundwater model objectives: characterisation and conceptualisation, design and optimisation, scenario analysis and impact analysis. The differences in model objective affect (1) the choice of a quantity of interest, (2) the balance between honouring observations, being consistent with system knowledge and estimating the range of model outcomes, (3) which sources of uncertainty to emphasize and (4) the trade-off between model runtime, number of parameters and number of model evaluations. These differences will ultimately affect which uncertainty analysis technique is most suited for a practical groundwater model investigation. The concepts are illustrated with a case study, designing the uncertainty analysis for an update to the groundwater model for the Angas-Bremer aquifer system in Australia.

The framework provides a way to systematically discuss, document and justify the various choices inherent to a groundwater model and uncertainty analysis and helps navigating the various uncertainty analysis approaches currently available.

# 1 Introduction

Uncertainty analysis in hydrogeological investigations and groundwater modelling has been a very active research topic over the last three decades. Despite, or maybe because of, this vast body of literature, practitioners still find it challenging in choosing an uncertainty analysis technique that is suited to their project objectives.

There are some excellent review papers and textbooks available that summarise the state-of-the-art in uncertainty quantification. Vrugt & Massoud (2019) for instance provides an overview of various uncertainty quantification techniques, with a focus on the Bayesian paradigm. The textbook by Scheidt et al. (2018) frames uncertainty analysis in Earth Sciences within a science-philosophical context and ties uncertainty analysis in with geostatistics and decision analysis. Classification of uncertainty analysis techniques in these texts is often based on the underpinning statistical paradigm and assumptions. Middlemis & Peeters (2018) for instance introduced this pragmatic, simplified classification:

1. Scenario-subjective

   A groundwater model is evaluated with a limited number of subjectively chosen parameter combinations. There is no formal uncertainty quantification, the results are often presented as 'sensitivity analysis' or accompanied by a subjective appraisal of probability (e.g. '*this parameter combination is extreme and not realistic*')

2. Deterministic-linear

   The model is assumed to behave linearly in the vicinity of a single parameter set that minimises the mismatch between observed and simulated values. Using linear error propagation equations, the uncertainty in parameters and observations, often described with multivariate normal distributions, can then be used to calculate the predictive uncertainty (White et al., 2014).

3. Stochastic-Bayesian

   While the groundwater model is still deterministic, the uncertainty analysis is based on the evaluation of an ensemble of parameter combinations, randomly sampled from posterior parameter distributions, i.e. parameter distributions that are constrained by historical observations through application of Bayes equation.

This classification provides a very high-level overview of the diverse approaches to uncertainty analysis, which makes it suited as an introduction to uncertainty analysis. However, it does not allow a nuanced appraisal of the differences between approaches, especially hybrid approaches that combine linear error propagation with a stochastic component. Heße et al. (2019) provides a much more elaborate, internally consistent, data-driven framework to guide discussion of uncertainty quantification in hydrogeology. The authors argue that the Bayesian approach, compared to other philosophies, is most suited for systematic uncertainty quantification. Nearing et al., (2016) provides a sound critique of the Bayesian approach for hydrological decision making and Nearing & Gupta, (2018) point to information theory as an alternative.

The objective of this paper is to help practitioners navigate this vast research field, not by starting from the theoretical foundations, but by pragmatically starting from the questions sought to be answered with uncertainty analysis. In this context, uncertainty analysis is defined here as:

*The research activity that seeks the range of model predictions that are consistent with observations and with system knowledge.*

Just as many model choices in a groundwater model depend on the objective of the groundwater model, the objective of the uncertainty analysis will determine choices such as which parameters to include or which uncertainty analysis technique to use.

The approach to navigating uncertainty analysis in groundwater modelling is summarised in Figure 1. This diagram is discussed in more detail in the next section, while the application section illustrates the concepts with a case study.

# 2 Methods

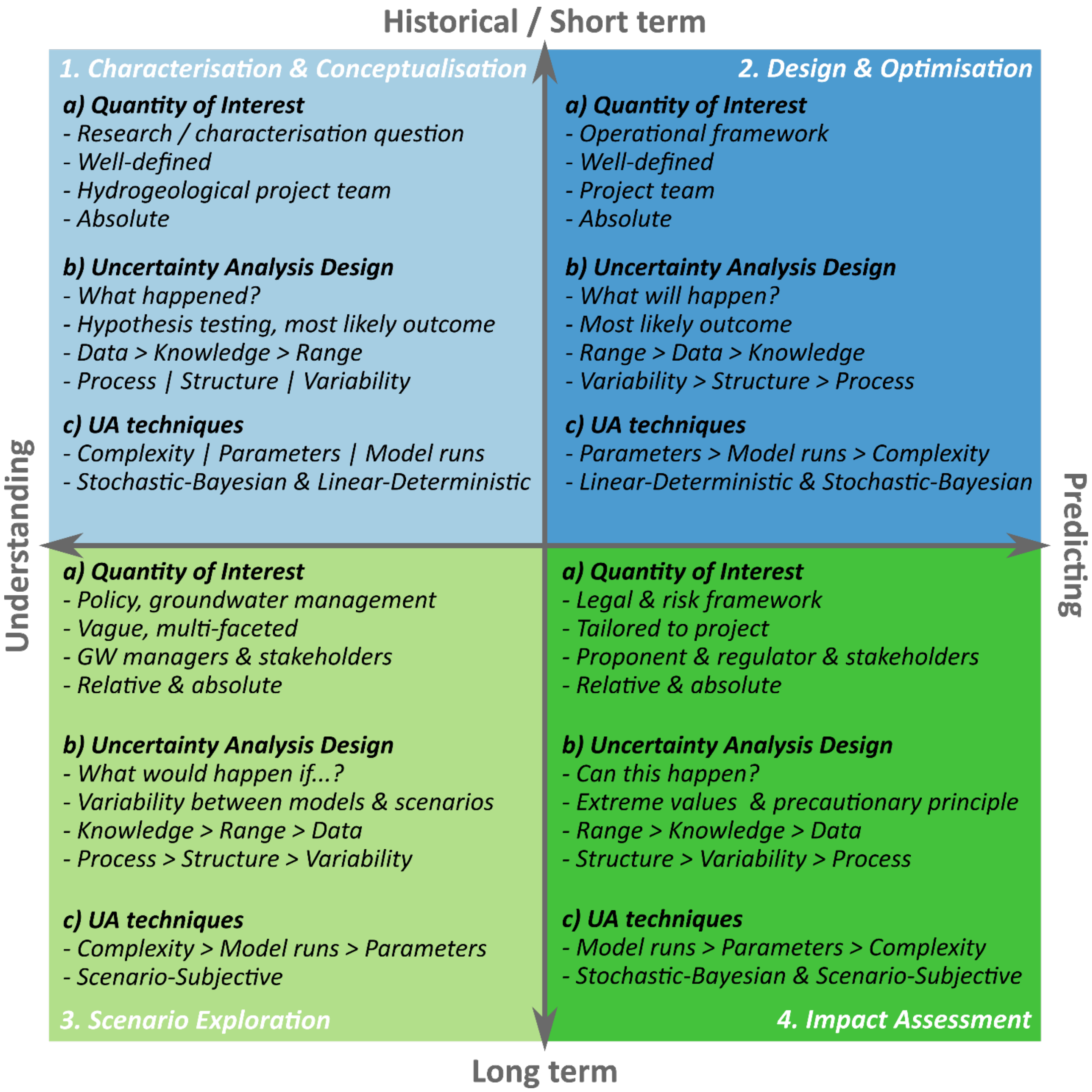


**Figure 1: The diagram summarizes four types of groundwater model objectives; 1. Characterisation & Conceptualisation, 2. Design & Optimisation, 3. Scenario Exploration and 4. Impact Assessment, in terms of a) the quantity of interest, b) requirements for uncertainty quantification and c) suitable uncertainty quantification (UQ) and sensitivity analysis (SA) approaches. The objectives on the left (pale background) have a focus on understanding the groundwater system, while objectives on the right (darker background) are more focussed on predicting future conditions. The time horizon for the objectives on the top (blue) is historical or short term, while the objectives on the bottom (green) have a longer-term time horizon.**

The diagram in Figure 1 is organised in four quadrants, corresponding to different types of groundwater model objectives:

1. Characterisation and Conceptualisation (CC):

   Characterisation studies estimate aquifer properties and boundary conditions (e.g. spatial distribution of hydraulic conductivity or recharge) while conceptualisation studies test conceptual hypotheses (e.g. Is a fault permeable? Is a river connected to the aquifer?). The focus is on understanding the groundwater system and reproducing historical observations.

2. Design & Optimisation (DO):

   Design and optimise infrastructure works (e.g. mine dewatering, tunnel inflow), groundwater remediation or irrigation schemes. The emphasis is on predicting rather than understanding and the time horizon is relatively short, measured in years rather than decades.

3. Scenario Exploration (SE):

   Inform groundwater management strategies and policy by evaluating groundwater management scenarios or future conditions, such as changes in land use or climate. The time horizon for predictions is often expressed in decades, with a focus on understanding the cumulative effect of multiple stresses.

4. Impact Assessment (IA):

   Evaluates the potential effect of a proposed development, such as water extraction for drinking water supply or for mine dewatering. The time horizon for predictions is often expressed in decades with a focus on predicting potential adverse impacts, often within the legislative framework of an environmental impact assessment.

The diagram in Figure 1 is not meant to be mutually exclusive. In analogy with geochemistry, it rather represents four different endmembers of groundwater model objectives where a groundwater modelling study can align to varying degrees with one or more of the types of model objectives. The diagram is intended to initiate and structure a discussion on how to deal with uncertainty in the early stages of a hydrogeological project. The discussion of the differences and similarities between the endmembers are organised in the following sections according to:

a) Quantity of Interest: how to choose the model output that will address the model objective;

b) Uncertainty Analysis Design: which aspects of the uncertainty analysis are most important for the model objective;

c) Uncertainty Analysis (UA) approaches: which uncertainty analysis technique to choose.

## 2.1 Quantity of Interest

The previous section discussed the various objectives of groundwater models. No groundwater model can however directly answer these objectives. The objectives need to be made explicit in space and time as a quantity of interest (QoI). This is the single model output or set of model outputs that are used to address the objective. For example: a suitable quantity of interest for the objective 'What is the impact of mine dewatering?' would be 'The maximum drawdown in monitoring bore X'.

A more formal definition of quantity of interest is:

*'A model state variable or derivation of a state variable, aggregated over a defined spatial and temporal extent.'*

A model state variable is any quantity computed by the numerical model, such as pressures, fluxes or concentrations. To make the QoI explicit in space and time, they need to be defined as a point in space and time (e.g. groundwater level at monitoring bore x at time y) or aggregated in space and time (e.g. average annual groundwater evaporation over polygon x).

The quantities of interest for CC, DO and IA studies are mostly well-defined as they are often directly specified through respectively the research question, the operational requirement or the legislative framework. An example for a Design & Optimisation study is a mine dewatering project, for which the quantity of interest is the timeseries of groundwater inflow into the mine pit as the mine progresses. An example for Characterisation & Conceptualisation is a pumping test where transmissivity and storativity in the vicinity of the pumping well are the quantities of interest. The objectives of Impact Assessment studies are intrinsically linked to the legal risk frameworks of the impact assessment. The quantity of interest is often directly defined through this legal risk framework. Examples are the maximum amount of drawdown permissible in an existing bore or a concentration threshold that cannot be exceeded. Defining a quantity of interest is however not always that straightforward or trivial. This is especially the case for Scenario Exploration studies, where objectives are often described in vague, multi-facetted terms, such as sustainability or aquifer conditions. A quantity of interest is often not unambiguously defined at the start of the project. On the contrary, these models are often used to explore which state variables are most sensitive to the various scenarios.

Tailoring the QoI to the project highlights another dimension to consider: who is involved in selecting the quantity of interest? For Characterisation and Conceptualisation, the quantity of interest selection is mostly done by the hydrogeological and modelling project team. In Design and Optimisation, technical experts from other domains may be involved, but the discussion is likely to be still limited to the project team. This is no longer the case for the Impact Assessment and Scenario Analysis, where actors outside the project team generally are involved. For Impact Assessment there are often three groups of people involved; the proponent who is submitting a proposal for a development, the regulator, the authority granting a license to operate and finally, stakeholders, representatives of other users that potentially be affected by the development. Scenario Analysis is often driven by a groundwater management team who will consult with the various stakeholders that use or rely on the groundwater system.

A final aspect to consider is to express the QoI as an absolute or relative quantity; i.e. as a state variable or as a change in a state variable compared to a reference condition. An example of an absolute QoI is a future groundwater level, while an example of a relative QoI is future drawdown, i.e. the difference between a future groundwater level and a historical reference groundwater level. A relative QoI has the distinct advantage that the predictive uncertainty is generally less than for an absolute QoI as uncertainties affecting both the prediction and the reference condition tend to cancel out. Relative QoIs also have the advantage that it is possible to attribute a change in state variable to a stress in the model. For instance, it allows statements such as ‘10% of drawdown at observation bore L is due to pumping from production bore A’. This is not possible with an absolute QoI. An absolute QoI however has the distinct advantage that it can be measured directly. A predicted groundwater level can be verified directly. A drawdown prediction can only be verified by taking into account both the reference level and the measurement.

For both the Design & Optimisation and for the Characterisation & Conceptualisation quadrants, the QoI tends to be absolute; estimating the historical or predicting the future condition of a state variable. QoIs for Impact Assessment and Scenario Analysis can be absolute, especially when there is a legally defined threshold or a historical reference condition. For those two quadrants however, the emphasis is often on comparing one or more possible futures, which favours relative QoIs.

## 2.2 Uncertainty Analysis Design

The previous section discussed how the outcomes of the groundwater model can address the model objective. In this section we look at how the uncertainty analysis can help in addressing the model objective. To start thinking about this, we illustrate each model objective with a relevant uncertainty analysis question:

1. Characterisation & Conceptualisation: What happened?
2. Design & Optimisation: What will happen?
3. Scenario Exploration: What would happen if …?
4. Impact Assessment: Can this happen?

These questions may look very similar, but they highlight some subtle, yet important differences and similarities.

For Characterisation and Conceptualisation, the focus is very much on the past, trying to reproduce and understand past events and observations. The outcome of an uncertainty analysis for characterisation questions the most likely model outcome is often preferred, while for a conceptualisation question it is the probability with which a hypothesis can be rejected.

The other three objectives are more forward-looking. In Impact Assessment, the potentially adverse effect of a development is at the forefront and the question to address and becomes almost binary; can an impact occur or not? As an outcome of the uncertainty analysis the most likely model prediction is not so much of concern, the focus is rather on the extreme values. It is in this context that the precautionary principle comes to the fore, ensuring impacts are overestimated.

The questions for Scenario Exploration and for Design and Optimisation are more open ended; ‘what would happen if…?’ and ‘what will happen?’ respectively. This phrasing emphasises that in Scenario Exploration the difference between scenarios if of most interest, while for Design and Optimisation studies, the most likely outcome within the development or management scenario is of most interest. The questions also highlights that in such studies, the development or management scenario itself is often not considered part of the uncertainty analysis.

The definition of uncertainty analysis in the introduction has three main components; the range of outcomes, consistency with the current state of hydrogeological knowledge and consistency with available historical observations. Figure 2 illustrates the trade-off between observations, knowledge and range of model outcomes for the four groundwater modelling objective endmembers.

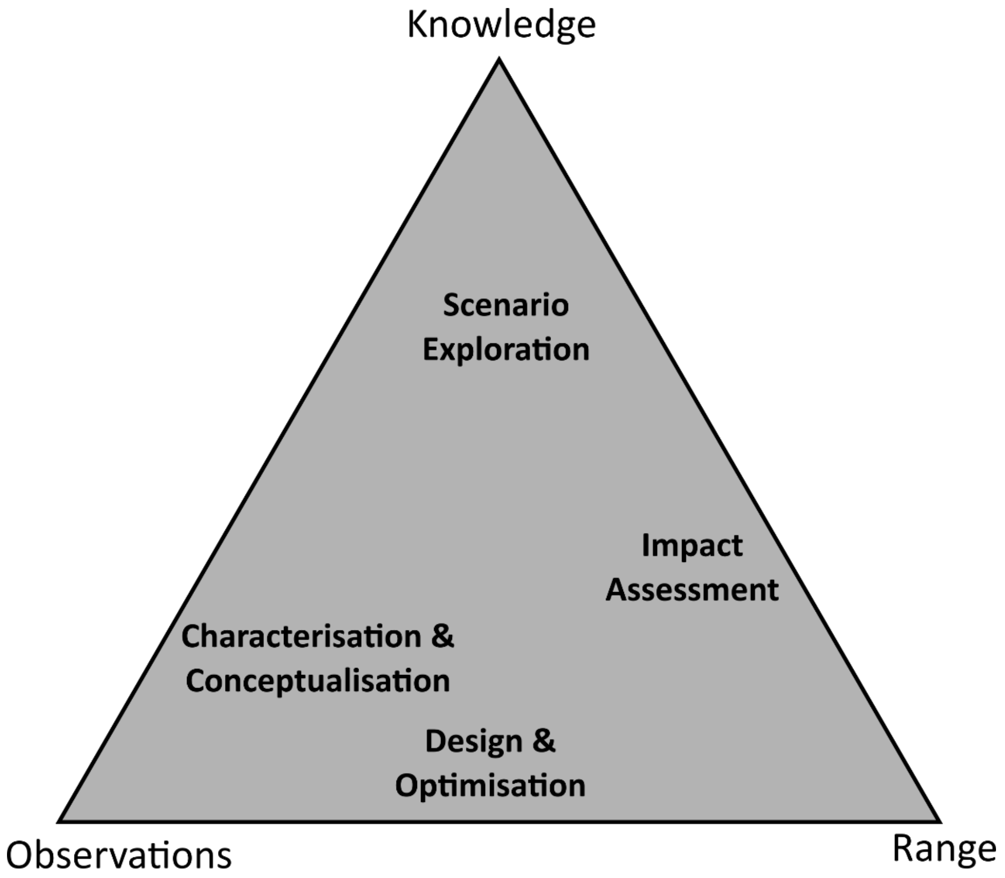


**Figure 2 Trade-off between range of outcomes, reproducing data and consistency with existing knowledge for the four groundwater model objective endmembers**

In Characterisation and Conceptualisation, the focus is on consistency with observations. This is the inference problem, in which the hydrogeologists wants to gain knowledge from observations. Consistency with existing knowledge is therefore also important; most progress in system understanding is made by reconciling observations that conflict with each other or with the prevailing understanding. The range of possible outcomes is considered least important in this kind of study.

In Impact Assessment however, the main emphasis is on the range of outcomes, especially the extremes of the range as the question to answer is ‘Can this happen?’. Consistency with existing knowledge is ranked higher than consistency with available data. In Impact Assessment, communication and the development of a narrative is key (Ferré, 2017; Bode et al. 2018). To have confidence in the range of model outcomes, stakeholders need to be presented with a logical narrative consistent with existing knowledge, of which matching historical observations is only a part.

This emphasis on existing knowledge is even more important in Scenario Exploration. The goal of Scenario Exploration is to find out what can possibly happen to gain additional insight into the groundwater system. As external stakeholders are involved in such studies, development of a narrative is paramount as well. The modelling team needs to show that historical observations are matched for the right reasons.

In Design and Optimisation, matching historical observations becomes more important, but remains second to estimating the potential range of outcomes. The focus is very much on prediction, hence the emphasis on the range of outcomes. Matching observations can greatly constrain relevant parameters, especially when observations similar to the prediction are available and the predictions are short term.

Before expanding on how the difference in emphasis in the uncertainty analysis will influence the choice of uncertainty analysis technique, another dimension needs to be considered in the design of uncertainty analysis; the different sources of uncertainty. Enemark et al. (2019) organises sources of conceptual uncertainty as those associated with (1) the representation of processes, (2) the geological structure (3) the spatial variability of properties. Representation of processes captures all lateral and internal boundary conditions, the fluxes in and out of the model domain. The geological structure pertains to how the hydrostratigraphy of the study area is incorporated in the vertical discretisation while spatial variability is related to the way spatial heterogeneity in hydraulic properties is simulated. Figure 3 shows our interpretation of the dominant source of uncertainty for each of the four groundwater model objective endmembers.

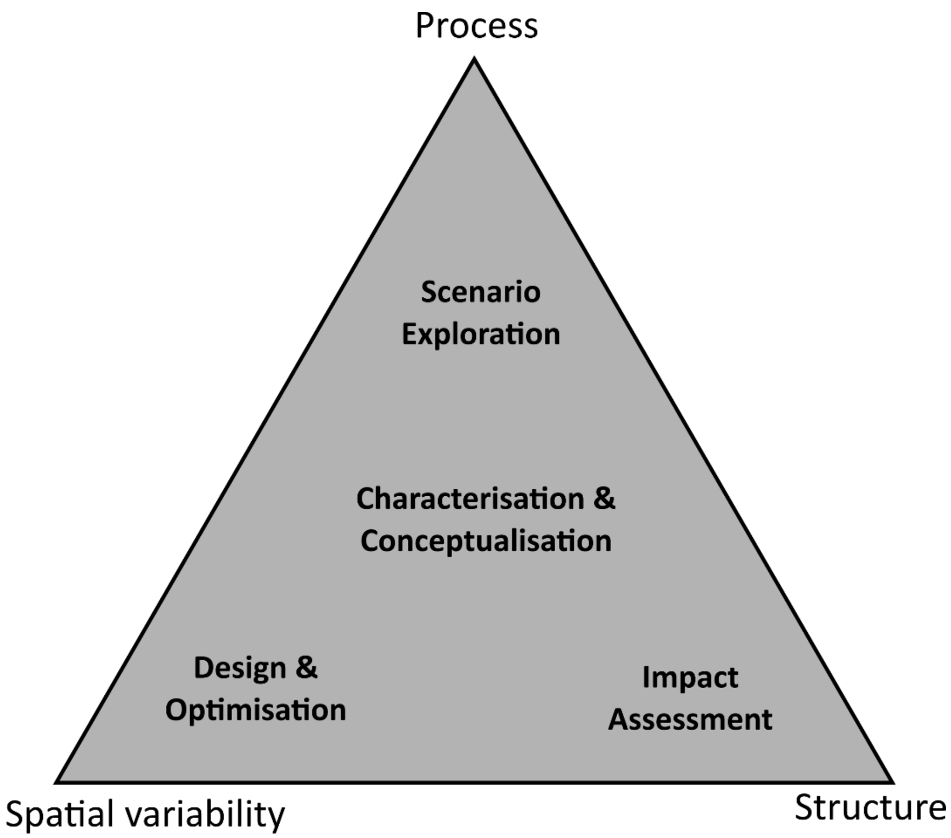


**Figure 3 Dominant source of uncertainty (process, spatial variability and structure) for the four groundwater model objective endmembers**

In Scenario Exploration, process uncertainty is considered the dominant source of uncertainty as scenarios often have differences in the fluxes in or out of the model. Examples are an increase in pumping or a reduction in recharge due to land use change. For Impact Assessment, structure is ranked as dominant source of uncertainty, followed by spatial variability and process representation. The processes affected by the development are mostly well-known and impact of a development on pressures, fluxes or concentrations often depends on the degree of connectivity between the stress and the receptor. Connectivity is dominated by structural features such as the presence of an aquitard or an impermeable fault. The uncertainty in Design & Optimisation studies is often dominated by spatial heterogeneity in the vicinity of the development, for instance the remediation of a contaminated site or the inflow to a tunnel. Characterisation and Conceptualisation traditionally focus on spatial heterogeneity, but each source of uncertainty is ranked equal as all of them can be the subject of the characterisation or conceptualisation question.

## 2.3 Uncertainty Analysis Approaches

In a very practical sense, the choice of uncertainty quantification approach depends on the computational budget, both cost and time, available to the project. It is a trade-off between the run-time of the model, the number of model evaluations required for the uncertainty quantification and the number of model features included in the uncertainty quantification. A more complex model generally takes longer to develop and has a longer runtime and in a similar vein, a more comprehensive uncertainty quantification technique requires more model evaluations. The number of model evaluations required also scales with the number of model features included in the uncertainty quantification.

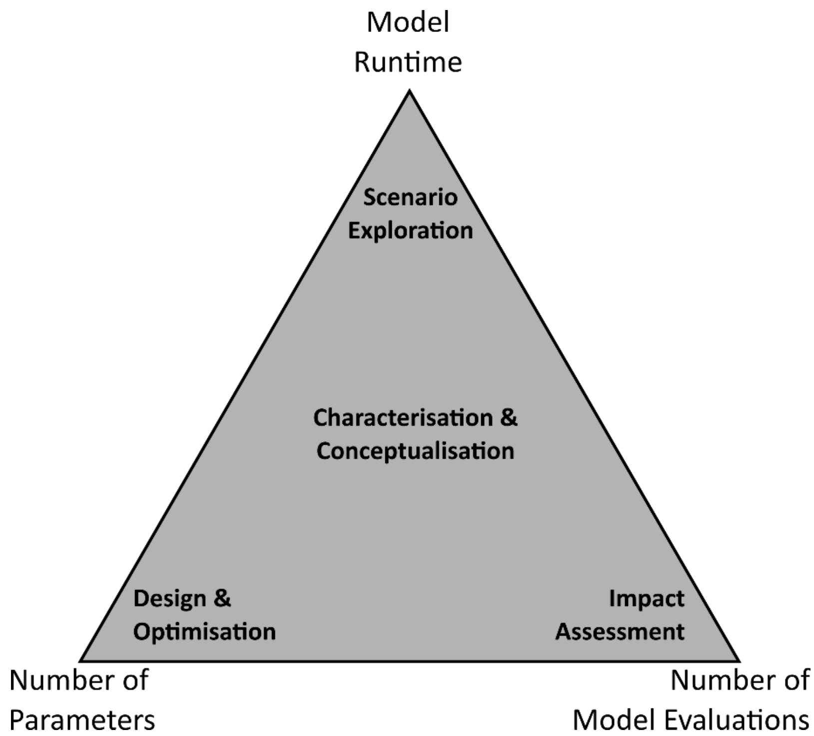


**Figure 4 Trade-off between model runtime, number of parameters and number of model evaluations for a fixed computational budget, for the four groundwater model objective endmembers.**

Figure 4 illustrates this trade-off between model complexity, number of parameters and number of model evaluations for a fixed computational budget with a ternary diagram. The different model objectives can be positioned in this diagram based on the discussion at the end of the previous section. For Impact Assessment it is most important to ensure the extremes of the ranges are captured. This can be achieved by increasing the number of model evaluations when sampling parameter distributions. Design and Optimisation studies benefit most from a detailed representation of spatial variability, which requires a large number of parameters. The largest source of uncertainty in Scenario Exploration pertains to process representation, which may necessitate a more complex model. Finally, Characterisation and Conceptualisation is placed in the middle of the diagram. Focus in this objective is on reproducing historical observations, which requires a comprehensive sampling of a model designed and parameterised to reproduce observations in an unbiased manner.

Model emulators or surrogate models (Asher et al., 2015) drastically reduce model run-time by replacing the original model with a statistical model that is trained on a set of model evaluations of the original model. As a rule of thumb, the accuracy of an emulator increases with the number of model evaluations used in training the emulator. The overall computational budget when using emulators can therefore be still high. One of the obvious drawbacks of emulators is that they are only reliable within the range of parameters and stresses included in their training dataset.

In the introduction, we presented the classification of uncertainty quantification techniques by Middlemis and Peeters (2018). Table 1 evaluates for each class of uncertainty analysis approaches if it can address the different objectives of uncertainty quantification; i) being consistent with existing knowledge, ii) reproducing historical observations and iii) providing an unbiased and accurate range of predictions. For completeness, we added qualitative uncertainty analysis (Peeters, 2017) as a separate entry. Qualitative uncertainty analysis is a systematic approach to discussing the rationale behind model assumptions and model choices and their perceived effect on predictions.

**Table 1 Evaluation of different uncertainty analysis approaches; Can they can guarantee achieving the components of the uncertainty analysis definition?**

| Components of uncertainty analysis definition | Qualitative uncertainty analysis | Quantitative uncertainty analysis | | |
|---|---|---|---|---|
| | | Scenario - subjective | Deterministic - linear | Stochastic - Bayesian |
| Consistent with knowledge | Yes | No (1) | No | No |

| | | | | |
|---|---|---|---|---|
| Reproduce historical observations | Not Applicable | No | Yes | Yes |
| Capture range and extreme values | Not Applicable | Yes (2) | No | Yes (3) |

(1) The limited number of model results does however allow in-depth inspection of potentiometric maps, time series and water balances

(2) Only if the parameter combinations chosen can be shown to result in an extreme prediction

(3) Provided it can be shown that i) all relevant sources of uncertainty are included, ii) the prior parameter distributions are informed or can be constrained by prediction-relevant observations and iii) the sampling of the posterior distribution of the quantity of interest is shown to converge for extreme moments

Only qualitative uncertainty analysis directly and explicitly evaluates if the model is consistent with existing knowledge. While the other methods embed existing knowledge in their initial parameterisation and regularisation, consistency with existing knowledge of the final parameter sets is only formally evaluated through how well the model reproduces historical observations. In Scenario Analysis with subjective probability, the model is only evaluated a small number of times. This allows inspection of modelled potentiometric or concentration maps, hydrographs and water balances in great detail. Such visual inspection often serves as a reality check for consistency with current knowledge of the system. In linear analysis and stochastic analysis it is often harder to do such an in-depth inspection of model outputs because of the large dimensionality of the output (ensembles of model output or mean and standard deviation).

Linear and stochastic analysis however do have the advantage that they are designed for inference; to find the parameter sets that are able to reproduce historical observations. In linear analysis the emphasis is on finding the parameter set that best fits the data, while in stochastic analysis there is a stronger emphasis on finding all parameter sets that match the historical observations. Scenario analysis with subjective probability is often based on manual calibration. There is therefore no guarantee that the parameter set minimises the model to measurement misfit or that the set of parameters evaluated in the scenario analysis represents the range of parameter sets that fit the historical observations.

Per definition, a qualitative uncertainty analysis as such does not quantify the degree to which historical observations are reproduced or the range of outcomes. It does however complement the other techniques when assessing if the approach captures the range of possible model outcomes and predictions.

Linear analysis does not guarantee an accurate range of predictions. The method relies on the model behaviour to be linear in the vicinity of the optimal parameter set and that both model parameters and predictions have a normal or log-normal distribution. It is difficult to show that these assumptions are valid for a model. The output of such analysis should therefore be considered as an indication of the order of magnitude that the range of predictions can span. This can be still useful, especially in Design and Optimisation studies, when we are interested in the most likely outcome and order of magnitude of uncertainty to establish a safety margin.

Much of the theoretical development in stochastic methods with Bayesian probability are focussed on the sampling of the posterior distributions, ensuring that the final ensemble is an accurate representation of all parameter combinations that are able to reproduce the observations. This however comes with an important caveat, as outlined in footnote 3 in Table 1; the qualitative uncertainty analysis needs to show that i) all relevant sources of uncertainty are included, ii) the prior parameter distributions are informed or constrained by prediction-relevant observations and iii) the sampling of the posterior distribution of the quantity of interest is shown to converge for extreme moments. In this last condition a moment means a summary statistic of the distribution, for instance the 95$^{th}$ percentile. Convergence of an extreme moment, for instance the 95$^{th}$ percentile, means that if more parameter values of the posterior distribution are evaluated, the value of the 95$^{th}$ percentile does no longer change. When these conditions can be shown to be satisfied, stochastic analysis can be very powerful for studies interested in extreme values, such as impact assessments. If extreme values are the sole interest however, it is more efficient to use a scenario analysis approach where the parameters are chosen such that they will lead to an extreme outcome. It is however not always trivial to select these parameter combinations from first principles.

**Table 2 Overview of which uncertainty analysis technique is suited for the four groundwater model objective endmembers**

| | | Quantitative uncertainty analysis |
|---|---|---|

| Groundwater model objective endmembers | Qualitative uncertainty analysis | Scenario - subjective | Deterministic - linear | Stochastic - Bayesian |
|---|---|---|---|---|
| Characterisation & Conceptualisation | Yes | No | Yes (most likely value) | Yes (hypothesis testing) |
| Design & Optimisation | Yes | No | Yes | Yes |
| Scenario Exploration | Yes | Yes | Yes (limited added value) | Yes (limited added value) |
| Impact Assessment | Yes | Yes (extreme parameters) | No | Yes (simple model) |

Table 2 shows an overview of which class of uncertainty analysis technique can be applied for the groundwater model objective endmembers. Qualitative uncertainty analysis, i.e. transparently discussing and justifying model choices and assumptions, is applicable to all objectives and should be an integral component of any groundwater model report.

Scenario analysis with subjective probability assessment is not suited for CC and DO, mainly because it cannot guarantee that the parameter combinations are consistent with the observations. It can however be useful in scenario exploration, where it will allow to rapidly evaluate different plausible scenarios. In impact assessment this approach can be used, only if it can be demonstrated that the parameter combinations chosen will result in an overprediction of impact such that the precautionary principle can be invoked with confidence.

As linear uncertainty analysis techniques assume the parameter set used for prediction is the most likely parameter set, deterministic models with linear uncertainty analysis are most suited when the accurate estimation of the most likely value of parameters is important, which are mostly the objectives CC and DO. Linear uncertainty analysis can be applied in scenario exploration, but it would need to be computed for each scenario. If the difference in predictions between scenarios is large compared to the uncertainty within a scenario, this approach will provide limited added value compared to subjective scenario analysis. This is mainly because of the additional computational requirement. Linear uncertainty analysis is not generally suited for impact analysis as it is very difficult to demonstrate that the linearity and normality assumptions hold and result in an accurate representation of the range of model outcomes.

Stochastic modelling with Bayesian uncertainty quantification can be applied to all types groundwater model objectives. The large computational demand of this approach will make the technique less preferred for applications such as design and optimisation or scenario exploration. In impact assessment stochastic modelling is most powerful when it is combined with a model in which only the complexity relevant to the prediction is retained (Schwartz, et al. 2017). Such a simpler model will generally have a shorter runtime, which allows a more comprehensive sampling of the parameter posterior distributions.

# 3 Case study

The framework presented in Figure 1 summarises the many dimensions of uncertainty analysis in groundwater modelling. In the next section we illustrate this framework in the context of a set of potential groundwater management challenges of the Angas-Bremer Prescribed Wells Area in South Australia, Australia (Figure 5).

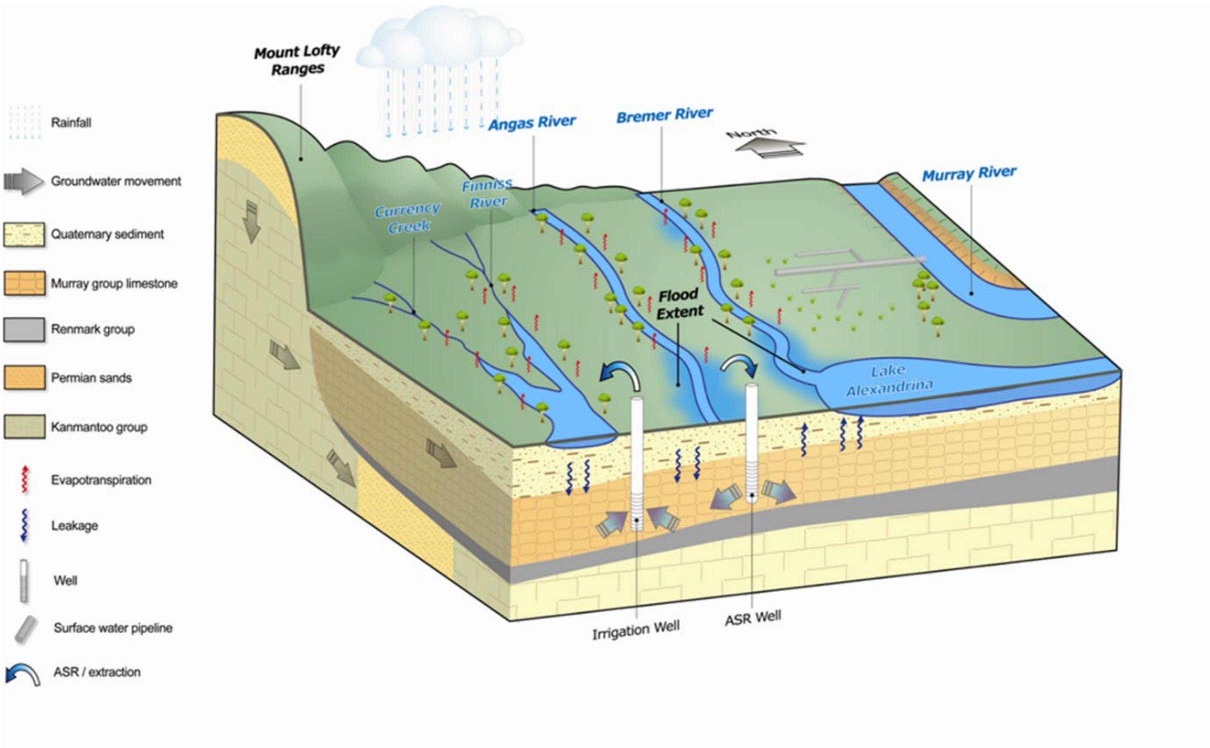


**Figure 5 Conceptual block diagram of the Angas-Bremer Prescribed Wells Area** (after Aquaterra, 2010)

Situated 70 km south of Adelaide, the aquifer system that underlies the catchments of the Angas and Bremer River supports an irrigated viticulture industry (Zulfic & Barnett, 2007). The main aquifer is the confined Murray group limestone confined aquifer, which is overlain by a semi-confined Quaternary aquifer. Recharge of the Murray group limestone aquifer occurs as (1) mountain-block recharge from the Mount Lofty Ranges Precambrian metasediments, (2) downward leakage from the overlying Quaternary aquifer. Groundwater discharge occurs to Lake Alexandrina in the south and through groundwater evaporation. Historical groundwater extraction for irrigated agriculture has caused salinity increases in the confined aquifer system due to downward leakage, to the extent that alternative surface water sources were developed, including pipelines from the nearby Lake Alexandrina and River Murray. Currently a number of aquifer storage and recovery installations are active to optimise water availability and manage salinity levels in the aquifer (Schulte & Cuadrado Quesada, 2020). In 2010, a groundwater flow and solute transport model was developed (Aquaterra, 2010). For the purpose of this paper, a hypothetical situation is considered in which groundwater management is interested in investing in an update of the groundwater model to address following groundwater management questions:

1. What is the dominant recharge process (Q1)?
2. How much of water injected during Aquifer Storage and Recovery (ASR) can be recovered (Q2)?
3. How will climate change affect groundwater conditions (Q3)?
4. Is the current level of groundwater extraction sustainable (Q4)?

The questions that will be discussed using the scheme outlined in the methodology are:

1. Quantity of interest: What should the modelling team focus on in the update of the groundwater model?
2. Uncertainty analysis design: Which sources of uncertainty need to be taken into account?
3. Uncertainty analysis approaches: Which uncertainty analysis technique will be the most cost-efficient?

## 3.1 Quantity of Interest

The four management questions each align with one of the quadrants in Figure 1. Identifying the dominant recharge process (Q1) is a characterisation and conceptualisation groundwater model objective, while Q2 is more aligned with design and optimisation. The climate change question

(Q3) is a scenario exploration groundwater model objective and the sustainability of current extraction (Q4) can be classified as an impact assessment groundwater model objective.

The research management questions are however quite vague and need to be made more explicit in a formal quantity of interest such that it becomes clear which groundwater model state variable and which model scenarios will be needed to address the management question. Table 3 provides an example of a formal quantity of interest for each of the management questions.

**Table 3 Examples of quantity of interest formulation or the Angas-Bremer management questions**

| | Management question | Quantity of Interest | QoI Type |
|---|---|---|---|
| Q1 | What is the dominant recharge process? | The volume of recharge over the study area from flood recharge and from diffuse recharge in the 2009 to 2019 period. | Absolute |
| Q2 | How much of water injected during Aquifer Storage and Recovery (ASR) can be recovered? | The maximum recovery volume that ensures stable or decreased salinity levels in the monitoring network after 10 injection-recovery cycles. | Absolute |
| Q3 | How will climate change affect groundwater conditions? | The difference in total volumes of recharge, pumping and aquifer storage over the study area between a 50-year future with historical climate repeated and a 50-year future with a different climate trend. | Relative |
| Q4 | Is the current level of groundwater extraction sustainable? | Does the difference of groundwater levels in existing bores at the start of irrigation season between a 30-year future with increased irrigation and a 30-year future with current level of extraction exceed the limit of acceptable change? | Relative |

Each of these QoIs identifies a state variable of a groundwater model, a temporal and spatial support (i.e. time period and area/location) and, for relative QoIs, the two scenarios that are compared. The QoI for Q2 is absolute (the recovered volume), but it can also be expressed as a relative QoI, for instance as the percentage of injected volume that can be recovered. The latter is most appropriate if more than one injection rate is considered. Unlike the other QoIs, the QoI for Q4 is expressed as a yes/no question as it is related to a limit of acceptable change. This limit of acceptable change is often determined in policy or legal frameworks that govern groundwater management.

## 3.2 Design of uncertainty analysis

In Figure 6, the four management questions are placed in the ternary diagrams that represent the trade-off between the range of outcomes, reproducing observations and consistency with existing knowledge (Figure 6a) and the trade-off between main source of uncertainties; spatial variability, process or structure (Figure 6b).

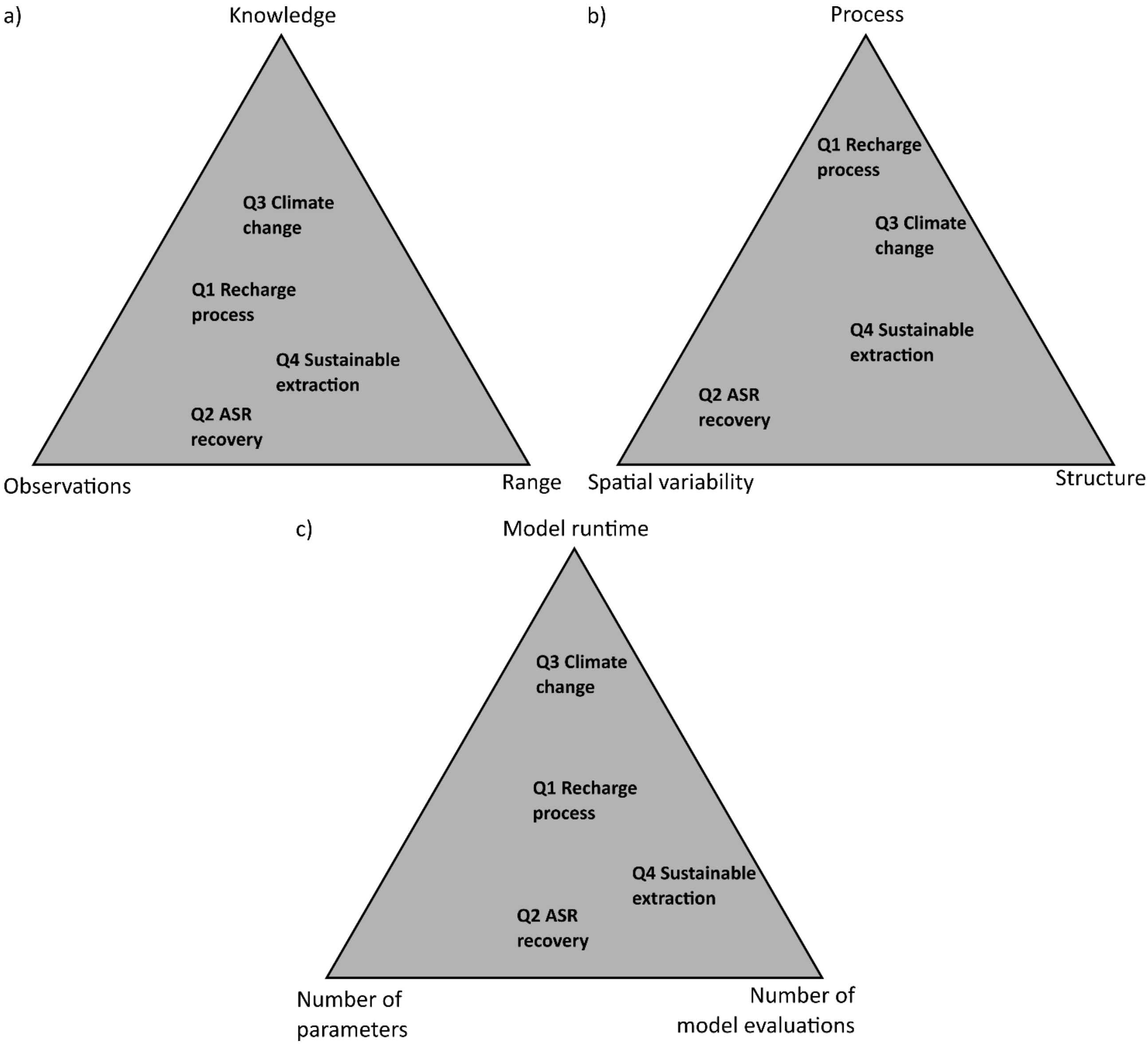


**Figure 6 a) trade-off between range of outcomes, reproducing observations and consistency with existing knowledge, b) trade-off in main sources of uncertainty and c) trade-off between model runtime, number of parameters and number of model evaluations for the four Angas-Bremer management questions**

For the Characterisation and Conceptualisation aligned question of identifying the dominant recharge process, reproducing historical observations is crucial to have confidence in the results of the modelling. There are however no direct measurements of recharge that can be used to calibrate the model. Inference of recharge with a groundwater model usually relies on measurements of other state variables, such as groundwater levels, surface water fluxes, or surface water/groundwater exchange fluxes (e.g. stream losses/gains or evapotranspiration from groundwater). To reduce the non-uniqueness such inference is prone to, the model needs to be constrained with other information from our understanding of the groundwater system. The range of model outcomes is not a priority, but determining which recharge mechanism is dominant requires comparing the distributions of simulated diffuse and local recharge. The main source of uncertainty for this QoI is process uncertainty; the implementation in the model of the recharge processes. Spatial variability can have a local impact but is likely of secondary importance for regional scale assessment of recharge fluxes. Recharge process focus on the shallow parts of the system, the structural representation of the deeper aquifers is therefore not a high priority.

The ASR recovery management question (Q2) is plotted near the bottom of the ternary diagrams. The most important dimension here is reproducing historical observations. ASR operations have been operational for several years in this region which means that there is a database of measurements that is directly relevant and informative for the QoI. Being consistent with existing knowledge is less important as informative calibration data is available. The range of outcomes, for instance confidence intervals, is important for management as it can inform the operational range of the ASR operation. Spatial variability is considered the most important source of uncertainty as the recovery of injected water is largely controlled by the hydraulic conditions in the immediate vicinity of the injection and recovery wells.

The climate change related management question (Q3) is plotted closer towards the knowledge endmember. The long time horizon of the prediction (50 years), historically unprecedented boundary conditions and focus on flux predictions, mean that the historical observational record is not likely to uniquely constrain the relevant parameters in the model. It will be therefore more important that the groundwater model reflects the conceptualisation of the system and its dynamics. The range of model outcomes is of secondary importance as it allows to compare the difference in model outcomes between scenarios with the difference in model outcomes within scenarios. The main source of uncertainty here is, like the recharge question, process representation. The effects of climate change will manifest themselves through a change in recharge processes, but also in changes in irrigated agriculture practices, which in turn may change groundwater extraction rates. As stresses can change both at the surface and deeper in the system, the representation of the structure, the connectivity of the aquifer systems will become important.

For the Impact Analysis related question on sustainable extraction (Q4), the range of model outcomes is by far the most important dimension. In a risk-based decision framework, the modelling needs to provide information to decision makers that the probability of exceeding the policy thresholds is at an acceptably low level. This requires a comprehensive assessment of the range of model outcomes. Reproducing with historical observations is slightly more important than consistency with existing knowledge in this case as length of the historical record is comparable to the prediction horizon (30 years) and the simulated stresses are comparable with historical stresses. The main sources of uncertainty for this management question are the representation of structure and spatial variability. The propagation of drawdown in an aquifer system is controlled by the connectivity between different aquifers or parts of aquifers and the bulk hydraulic properties of the aquifer.

## 3.3 Uncertainty analysis approaches

Figure 6c shows where the four management questions sit with respect to trade-offs in the implementation of an uncertainty analysis. The characterisation and conceptualisation management question to identify the dominant recharge process plots centrally in the ternary diagram. The model complexity needs to allow sufficient detail to represent the different recharge mechanisms. A more complex model tends to have a longer runtime and as a complex model has more degrees of freedom, the number of parameters to include in the uncertainty analysis increases. Identifying the dominant recharge process does not only rely on the most likely value for recharge volume for each process, but also on the range of values for each process. Accurately estimating such a range of outcomes requires a large number of model evaluations. For this management question it is recommended to select a Bayesian inference approach in which informative prior distributions are constrained by observations through a comprehensive sampling of parameter space, for instance through Markov Chain Monte Carlo.

The ASR recovery management question is an optimisation question that depends on local spatial variability. Accounting for spatial variability requires a large number of parameters, while an optimisation requires a large number of model runs. Model runtime is therefore preferably kept short, for instance by simplifying the representation of boundary conditions. Linear uncertainty analysis approaches and their non-linear variants are well suited to handle large numbers of parameters and efficiently arrive at an optimal parameter combination for prediction.

For the climate change management question, the emphasis lies on representing system knowledge and understanding. A more complex model allows for more detail in representing system knowledge, but the associated longer runtime will limit the number of parameters that can be included in the uncertainty analysis and the number of model runs that can be evaluated. Uncertainty analysis, either through linear or stochastic methods, is useful in this context to quantify the difference between the within-scenario variability and between-scenario variability.

As the goal of such exercises however is to increase understanding of the system, a limited number of carefully selected scenarios may be more informative and cost-effective. A limited number of model runs has the added advantage that the results can be examined in greater detail (potentiometric maps, hydrographs, water balances, etc).

The last management question on sustainable levels of extraction is an Impact Analysis groundwater model objective. The focus is on capturing the extremes of the range of outcomes which requires a comprehensive sampling of the model parameter space, which requires a large number of model evaluations. Model runtime can be decreased by only incorporating processes that are directly relevant for the QoI. The number of parameters can be reduced by limiting the spatial variability in hydraulic properties which is justified for regional scale predictions of drawdown as these dependent on the equivalent hydraulic properties between stress and prediction location rather than the local variability. Comprehensive stochastic sampling of parameter space is of utmost importance to estimate extreme predictions. If the system is not too complicated, such as in this case drawdown predictions in the same aquifer as the stress, it is possible to select which parameter combinations will lead to the most extreme prediction. A single model run, with carefully selected parameter combination, can then provide sufficient information to inform risk-based decision making.

Returning to the hypothetical question on where to invest when upgrading the groundwater for the Angas-Bremer region, it is apparent that a single upgrade of the existing groundwater model or a single approach to uncertainty analysis is not likely to satisfy all the requirements for the different objectives. The reasoning presented above can however be used in engagements with the funding bodies and other stakeholders as to where to prioritise groundwater model investment.

# 4 Discussion

The scheme we introduced here is not intended as a rigid classification rubric, like for instance the groundwater model confidence level classification of Barnett et al. (2012). On the contrary, it provides a framework to systematically discuss the various dimensions of groundwater modelling and uncertainty analysis. The emphasis should not be in where exactly a groundwater modelling question lands on the diagrams shown in Figures 1 to 4. The focus should be on the narrative, explaining and motivating the various trade-offs during modelling. The ability to explain these model choices is often more important to build trust with stakeholders in the model predictions than the complexity of the model or the statistical rigour of the uncertainty analysis (Ferre, 2020) .

As outlined in the introduction, there are several other texts that organise uncertainty analysis approaches, often based on the statistical underpinnings. Our scheme has more in common with the summary table in the paper of Doherty & Moore (2019) in which they argue for a more critical, prediction focussed approach in designing groundwater models and associated data assimilation and uncertainty analysis to inform decision making. The summary table provides an overview of which uncertainty analysis techniques are suitable as a function of data availability. Our framework expands on these ideas by not only considering how the groundwater model outcomes will inform decision makers, but also the various ways in which uncertainty analysis can inform decision makers.

The Angas-Bremer case study illustrates this clearly. Even with the same availability of data, the different research management questions not only require different approaches in groundwater modelling, they also require different approaches in uncertainty analysis. The only way that a single groundwater model with a single approach to uncertainty analysis will be able to address all the management questions, will be through an enormous investment of resources. Building different versions of a groundwater model for the region, tailored to the management question, with a suitable uncertainty analysis approach will be far more cost-effective.

# 5 Conclusion

This paper provides a pragmatic overview of aspects to consider when planning uncertainty analysis in a hydrogeological investigation, focussing on what you want to achieve with the investigation and what question you want addressed through uncertainty analysis.

The simple diagrams shown can never fully capture the complexity of this field and it is not intended as a rigid classification. It will however allow practitioners to frame their thinking and provide a roadmap to navigate the exciting but daunting world of uncertainty analysis.

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