Fate and transport modelling for monitored natural attenuation projects: what should be considered to maximise the value in decision making?

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Abstract The Cooperative Research Centre for Contamination Assessment and Remediation of the Environment (CRC CARE) identified the need for the development of a technical guidance document on assessment, implementation and verification of Monitored Natural Attenuation at sites with residual dissolved phase hydrocarbon impact in groundwater. As part of the development process there was a need to include guidance on fate and transport modelling as there was a lack of relevant guidance in Australia and industry practice varied widely. One key consideration in the development of guidance was consideration of what value fate and transport modelling adds to the decision making process, and what standards the models need to meet to produce reliable results within acceptable bounds of uncertainty. The guidance document considered the key elements that should be included in any fate and transport model, and how these address uncertainties and provide transparency on reliability of modelling results for consideration by stakeholders and decision makers on the applicability of Monitored Natural Attenuation.

Key words MNA; modelling; dissolved phase; guidance; uncertainty; Australia

INTRODUCTION

Understanding the likely future behaviour of dissolved phase hydrocarbon plumes is one of the main uncertainties associated with implementation of a Monitored Natural Attenuation (MNA) strategy (AFCEE, 1995; ASTM, 1998; EA, 2000). The Cooperative Research Centre for Contamination Assessment and Remediation of the Environment (CRC CARE) responded to a need for technical guidance by development of a national technical guidance document for implementation of MNA in Australia (McLaughlan *et al*., 2006). One of the aspects considered in the development of the document was use of the fate and transport modelling in project feasibility assessment and decision making on future plume behaviour.

While detailed guidance was beyond the scope of the final document, CRC CARE recognised a need for basic guidance on essential elements to be included in any fate and transport model.

Predicting the future behaviour of the plume may be required to ensure ongoing containment within acceptable boundaries and continued absence of risk to receptors (Bear & Verruijt, 1987; Anderson & Alhajjar, 1995). This may be achieved through robust monitoring over a sufficient period to provide confidence in the groundwater system dynamics. Alternatively, in situations where insufficient data or time is available, future plume behaviour can be predicted by a dedicated solute transport computer model. However, this latter approach has a number of limitations that need to be recognised and clearly understood by stakeholders to allow for sound decision making.

DEFINING MODELLING OBJECTIVES AND DATA COMPILATION

Developing appropriate objectives for the modelling is a key consideration in the successful demonstration of MNA viability (Domenico, 1987). Before undertaking any modelling, the objectives, purpose and benefits of undertaking the modelling need to be clearly defined (McAllister & Chiang, 1994; Einarson & Mackay, 2001; ITRC, 2009). The higher the accuracy of the site-specific parameter estimates, the lower the uncertainty associated with any numerical simulation developed based on these parameter estimates (Newell *et al*., 1995; Middlemis, 2001). One of the common issues encountered in numerical modelling to support MNA is use of standard / generic or cookbook-type model definitions, which often miss the subtleties and individualities of any site to which they are applied, leading to greater uncertainty and less defensible outcomes. Therefore, development of a site-specific tailored definition of the modelling objectives forms an essential foundation for any numerical simulation.

The data collected as part of the NA characterisation phase need to be carefully reviewed to establish their value to the modelling (Newell & McLeod, 1996), and the impact on uncertainty of outputs. Table 1 lists the parameters for which site-specific information is essential to model hydrocarbon impacts in groundwater systems.

Table 1 Typical data requirements for predictive solute transport models (modified from WSDE 2005).

Parameter	Aquifer depth/geology (1)	Hydraulic conductivity (2)	Hydraulic gradient and direction of flow (2)	Hydraulic head dynamics (3)	Porosity (1)	Transport porosity (1)*	Bulk density (1)	Dispersivity (1 + 2)*	Moisture content of unsaturated zone (1)	Vapour phase concentration distribution (1)	Fraction of organic carbon (1)	Rainfall, infiltration and recharge	Degradation rates[#]	Contaminant concentrations and delineations (1+2)	Biochemical environment (2)[+]	Vapour mass flux
Matrix	**E**	⊘	⊘	⊘	**D**	**U**	**D**	**D**	**D**	⊘	**E**	**D**	**D**	**E**	**D**	⊘
Solution	⊘	**E**	**E**	**D**	⊘	⊘	⊘	**D**	⊘	⊘	**E**	**D**	**D**	**E**	**E**	⊘
Vapour	⊘	⊘	⊘	⊘	⊘	⊘	⊘	⊘	⊘	**U**	⊘	⊘	**D**	**U**	⊘	**U**

Notes:
(1) Requires investigation bores and soil /rock testing
(2) Requires installation of monitoring wells and testing
(3) Seasonal, recharge, anthropogenic
* Difficult to establish requires long-term monitoring or tracer test
[#] Difficult and expensive to measure and requiring long-term monitoring. BUT vital to provide confidence
[+] Biodegradation indicators (pH, Eh, Temp, DO, Mn, NO_3, Fe, SO_4 and CH_4)
E = Essential
D = Desirable
U = Useful
⊘= Not Relevant

The quality and quantity of the available data should be taken into account when selecting the solute transport model (Spitz & Moreno, 1996). Distributed numerical models (finite difference or element-based codes) should not be considered where data are limited to the point where a high degree of uncertainty is associated with the predictions. Even when simple analytical calculations are used that require a single value for each parameter, those parameter values must be representative of the site and the area being modelled, and must be adequately justified.

Single site-specific measurements should be used with considerable caution because of the high level of uncertainty that can result. It should be recognised that some parameters will vary with location and depth on a site, and depending on the value selected, can potentially result in differences in model outputs by orders of magnitude. Selecting a single parameter value that is representative in this situation is a gross simplification and is one of the challenges of modelling.

Probabilistic model approaches can accept estimates of parameters in the form of a distribution; however, this does not eliminate the uncertainty in outcome associated with parameter estimates that happen to not appropriately represent the situation that applies. Particular caution is required if parameter distributions are literature-based, as variations of an order of magnitude or more can be common, and variations of this magnitude can result in a high level of uncertainty in predicted behaviour of a plume.

Using a robust, statistically-derived data set of site-specific parameters representative of the situation at the site is essential if the model outputs are to be reliable and to have an acceptable level of uncertainty.

CONVERTING A CONCEPTUAL SITE MODEL INTO A SOLUTE TRANSPORT MODEL

NA characterisation should result in a good understanding of the source and hydrogeological regime, and a conceptual site model that is able to account for the various observations relating to the distribution of contaminants and indicator parameters. This conceptual site model can form the basis for the solute transport model. The development of a solute transport model must consider and comment on:

- what is known and understood about the groundwater system and its interaction with the wider environment
- what components of the model are not known or not understood with sufficient confidence
- what the key physical and chemical processes are and how can they be represented
- what the assumptions are that need to be made for the model, and
- what data and components of the system can be ignored or simplified while still meeting the modelling objectives.

Conceptual models for computer simulation include qualitative and quantitative elements that describe the system to be simulated. The conceptual model for simulations should also consider the uncertainties in defining the system behaviour and how this affects the accuracy and uncertainty of predictions derived from the simulation.

Achieving a balance between simplification and complexity is an important aspect of the conceptualisation phase. Over-simplification results in a model incapable of adequately simulating observed conditions. Under-simplification results in a model too complex for efficient and cost-effective problem analysis, and can hinder the model in being a useful predictive tool. Any conceptual model will be imperfect and the key is managing the level of uncertainty.

MODEL SELECTION AND DOMAIN DESIGN

A wide range of modelling tools is available for simulation of petroleum hydrocarbon transport (WDNR, 2003; WSDE, 2005). No one modelling tool fits all situations, and selection of the model will depend on the following:

- what the modelling objectives are
- what components of the groundwater system are relevant to the model
- how the conceptualisation of the model will translate into the simulation domain
- what data is available in relation to the model input requirements
- what natural processes are being modelled
- what the model's capabilities and limitations are in dealing with the dynamics observed in the groundwater system being studied
- what the experience and preference of the person undertaking the modelling is and their personal preferences, which can limit the relevance of the model or acceptability to stakeholders.

The design of the model domain will be site-specific and model dependent (Zheng & Bennett, 1995; EA, 2001; Middlemis, 2001; WSDE, 2005). All models require the model domain to be specified, which as a minimum needs to include the size of the study area, source and area of contamination, location of receptors, presence of natural boundaries, such as the edge or limits of the geological formation or aquifer, faults, rivers, groundwater catchment divides and the dominant fate and transport processes controlling contaminant migration.

MODEL CALIBRATION, MODEL VERIFICATION AND VALIDATION

Once the solute transport model code is selected and the domain established, a numerical simulation needs to be set up using a set of input parameters that allows comparison of the model output to a known set of field observations to calibrate the model and confirm that the numerical simulation can adequately simulate the groundwater system being studied. Throughout the calibration process, the modeller must review model outputs in the context of the limitations of the definition of the system behaviour and the assumptions used in representing this system mathematically (Zheng & Bennett, 1995; Newel *et al*., 1996; Middlemis, 2001; WSDE, 2005). Calibration can be achieved by manual changes to input using a trial-and-error approach or automated calibration routines (e.g. PEST code for MODFLOW).

It is essential that the adjusted parameter values required to achieve calibration be compared with what can be expected to be representative of the hydrogeological regime for the site. It is often found that the parameter estimates necessary for achieving calibration are not representative, and such variations need to be reconciled with site observations. Also, a common issue, particularly in highly urbanised areas, is that the monitoring wells used are not on or near the plume centre line, thus causing uncertainty in relation to the reliability of the model predictions and maximum predicted concentrations.

Model verification and validation follows the calibration step and requires an independent data set from that used in the calibration (Zheng & Bennett, 1995; Middlemis, 2001). A model cannot completely duplicate historical data under all conditions due to it being just a mathematical representation of reality, model solutions not being unique, i.e. adjustment of one set of parameters can yield the same result as adjustment of another, unrelated set of parameters, and historical data contain problems with accuracy, precision and completeness.

Validity is a matter of degree that depends on the information available and the requirements established by the decision-maker. Model validation is almost always difficult, requiring a large amount of independent, high quality data, and hence is not commonly undertaken.

MODEL SENSITIVITY ANALYSIS

The purpose of undertaking a sensitivity analysis is to identify those input parameters that have the greatest influence on model predictions, and hence should be known as accurately as possible. The sensitivity analysis can assist in deciding whether further investigation is needed to better define these parameters (Zheng & Bennett, 1995; Newel *et al*., 1996; EA, 2001; Middlemis, 2001; WSDE, 2005).

While the model outputs can be highly sensitive to the values assumed for some parameters, in the case of other parameters the sensitivity of the model outputs may not be significant. In general practice sensitivity analysis is infrequently undertaken and this often limits the understanding of model representativeness and defensibility of outputs.

MODELLING SCENARIOS

Before commencing the simulation, the modeller should ensure the model can be expected to be able to simulate the natural system within an acceptable uncertainty range and confirm that the proposed model will be acceptable to the relevant stakeholders.

Because of the variety of scenarios that may need to be considered, providing guidance that will address all situations is difficult to develop (Zheng & Bennett, 1995; Middlemis, 2001). However, as a minimum a likely and worst case scenario should be considered. The likely case is based on analysis of the available data refined in matching modelled results with field data. The worst case prediction sets parameters at their most conservative, but within the bounds of the uncertainty around the parameters. The difference between a likely estimate and a worst-case prediction will provide an initial indication of the magnitude of uncertainty in the model results.

The results of these two basic modelling scenarios can then be compared to designated target or trigger values for the compliance points to assess viability of an MNA strategy for a given situation. Additional scenarios may be required depending on whether the two essential scenarios address the requirements developed and the project data quality objectives (DQOs) and modelling objectives. A key limitation of many models developed is the consideration of only a single scenario, which imposes limitations on the stakeholder's ability to understand the uncertainties in the predictions and understand their reliability and representativeness.

ACCURACY AND UNCERTAINTY OF MODEL PREDICTIONS

Understanding the uncertainty associated with the model predictions is an essential consideration in the application of a predictive solute transport model (Zheng & Bennett, 1995; Middlemis 2001). Uncertainty in model simulations results from:

– natural variability of aquifers' geological, hydrogeological and hydrogeochemical properties that translate to the adopted input parameter estimates
– source parameters can be difficult to define and options with most modelling packages are limited. Thus accurate simulation of natural systems and their source dynamics is often not feasible, resulting in the introduction of uncertainty
– variability between the transport mechanisms in the aquifer and the adopted mathematical equations chosen to simulate them
– various sink/source phenomena such as heterogeneity on mass loading within the source zone
– values of model coefficients and their spatial and temporal variation between the aquifer and model domain
– initial conditions adopted for the model
– the location of domain boundaries and the prevailing conditions
– the measuring accuracy of data employed in model calibration, and
– the ability of the model to cope with a problem in which the solid matrix heterogeneity spans a range of scales, sometimes orders of magnitude apart.

All models have inaccuracies and uncertainties, and thus all simulations need to be accompanied by an uncertainty analysis and error statement (Anderson & Alhajjar 1995; Zheng & Bennett, 1995; Middlemis, 2001). Errors can be expressed qualitatively, but preferably quantitatively. Stochastic models provide the ability to predict future plume behaviour at predetermined confidence levels; however, these will also have a degree of uncertainty and it should not be assumed that the results necessarily have a higher degree of confidence. The confidence levels need to be established in consultation with stakeholders to ensure the model outputs are acceptable.

Any modelling results presented without an uncertainty statement should be regarded with caution. For example, a model prediction that indicates simply that the maximum extent of the plume is yy metres and will occur in zz years would need to be questioned, and the possible range in values assumed for parameters such as hydraulic conductivity, head and rate of biodegradation would need to be compared with the values measured and possible at the site, and confidence gained that the possible range of outputs reflects this.

Particular caution should be taken with the reporting of model outputs in that once numbers are presented in a report, they tend to gain credibility and be quoted as fact. It should be remembered that they are at best approximate estimates and may have an order of uncertainty of possibly an order of magnitude, and should not be reported with more accuracy than is inferred from a single significant figure. This is one of the essential divides that occurs between proponents and regulators, which results in delays of implementation or rejection of MNA as an appropriate approach for dealing with residual dissolved phase hydrocarbon plumes.

UNCERTAINTY ANALYSIS

When studying natural systems through the collection of a range of single value parameter estimates and numerical simulations there is an inherent uncertainty in the decision-making process that has to be acknowledged and communicated. No investigation, however intensive, can fully define a natural system. Thus, uncertainty is an inherent part in the assessment of MNA viability assessment (Anderson & Alhajjar, 1995; Zheng & Bennett, 1995; Middlemis 2001). The key sources of uncertainty in any MNA viability assessment are:

Investigation location selection, sampling pattern and sample collection method All of these factors influence the level of information obtained from an investigation and the foundation of the conceptual model. Yet no system can be sampled sufficiently to fully characterise all of the physical and chemical properties to the point where there is no uncertainty in their spatial or temporal distribution.

Field/laboratory data There is inherent uncertainty in the point measurement of all field/laboratory data and in producing spatial distributions based on them.

Conceptual model The most serious cause of error in establishing MNA viability arises from deficiencies in the formulation of the conceptual site model for the site and numerical simulations. The conceptual model is a simplified description of the real aquifer system. Alternative conceptual models can be formulated, which are equally plausible, so that both require testing. This is commonly called conceptual uncertainty.

Modelling package selection All modelling software has limitations that need to be understood in order to factor these into the uncertainty analysis. This applies from simple analytical models to more advanced numerical simulations.

Model input data There are errors introduced due to the uncertainty in the model input parameters adopted. Model parameters are applied to cells or zones across which the properties are averaged, thus not representing the real heterogeneity of the system. This is very scale dependent so greater accuracy requires much greater detail.

Mathematical representation There will be inherent errors associated with the mathematical representation of the physical processes (e.g. the governing equations and boundary conditions are simplified mathematical descriptions of the conceptual model). In addition, the numerical approximations used to solve these equations and the associated spatial and temporal resolution introduces further errors.

Predictive uncertainty There will be errors in the model predictions because future conditions are estimated but will in reality be different.

Any MNA viability assessment must be accompanied by an outline of uncertainty associated with the results, including the significance of the uncertainty in terms of the project DQOs, the modelling objectives and the viability of an MNA strategy.

CONCLUSIONS

CRC CARE responded to a need for guidance ion MNA implementation by development of a national technical guidance document for Australia. This included consideration of guidance on fate and transport modelling, since there was limited guidance on this aspect available in Australia, and included consideration of:

- Data compilation and requirements considered essential for development of representative models, use of probabilistic models and the effect of data uncertainty on model outcomes;
- Conversion of conceptual models to numerical representations and how simplification affects model accuracy and representativeness;
- Model selection and domain design that may be utilised for the numerical simulation and how to design the domain to be representative of the situation being simulated;
- Model calibration for achieving calibration, considering acceptable uncertainty and stresses the need to consider representativeness of the data once model calibration is achieved;
- Model verification and validation to independently verify and validate model performance;
- Model sensitivity analysis outlines the need to consider the sensitivity of the numerical simulation to variance in the input parameters and is a major contributor to understanding which data is critical to model stability and representativeness.
- Modelling scenarios set out requirements such as the model being able to replicate the natural environment simulated to within an acceptable degree of accuracy and that the model scenarios proposed are acceptable to stakeholders before modelling commences. Also set out is a minimum requirement for a likely and worst case scenario highlighting that single scenario simulations offer little value.
- Accuracy and uncertainty of model predictions outlines the common causes of uncertainty in model predictions, covering issues such as mathematical simplifications, heterogeneity, source behaviour, initial conditions, boundary conditions, etc. The document stresses that all models no matter how sophisticated have uncertainty and this must be understood and represented in the model results documentation.
- Uncertainty analysis. This final step outlines the need of integrating the modelling results with the wider MNA project decision making and stresses the need to clearly understand and communicate the inaccuracy of the model, and the effects this has on the uncertainty in the overall MNA project decision making.

Therefore, in summary, use of numerical modelling is often an integral part of MNA projects. This paper illustrates that provided sufficient robust work backed by adequate documentation is undertaken the modelling can add considerable value to the overall decision making process (Wiedemeier *et al*., 2000). However, experience by the authors has demonstrated that when modelling is over-simplistic, poorly documented or undertaken in isolation, the associated uncertainty limits, detract from, or at times reverse the value provided by the model to the decisions that need to be made. Therefore CRC CARE included basic guidance on the key elements and considerations for numerical modelling as part of MNA projects to improve the overall application across the Australian contaminated land assessment practices for MNA projects.

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