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**Best Management Practice
for Developing Remedial Action Plans
Based on Numerical Modelling Approaches**

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1.0 INTRODUCTION

The Alberta Tier 1 and Tier 2 guidelines (AEP, 2019a,b) are a convenient and widely used screening-level approach for developing remedial programs that will meet the goal of avoiding adverse effects for valued receptors. These guidelines consider a range of exposure pathways including groundwater-mediated pathways. The Tier 1 and Tier 2 models take a simplified approach to calculating remedial guidelines for groundwater pathways by assuming that the chemical is present at uniform concentration within a rectangular cuboid of specified length, width and thickness.

In reality, contaminant plumes have concentration profiles that vary spatially in three dimensions, and rarely, if ever resemble a uniform cuboid. By assuming a uniform cuboid of uniform contaminant concentration, the Tier 1 and Tier 2 models will always overestimate the contaminant mass present in a system. Practical experience with assessing real plumes suggests that the magnitude of this overestimation of contaminant mass is typically 1 to 2 orders of magnitude, depending on the complexity and shape of the plume. When these guidelines are used to inform remedial action plans, this overestimation of mass will result in more remediation than is necessary to achieve remedial goals in cases where those goals are driven by groundwater-mediated pathways.

At smaller and simpler sites, application of Tier 1 and Tier 2 will often be the most effective way to proceed, as the significant additional level of effort required to account for the actual distribution and movement of contaminant mass may not be justified. However, the over-remediation associated with the application of Tier 1 and Tier 2 guidelines can become a major impediment to developing an economically viable remedial plan at large and complex sites where groundwater pathways are the drivers for large remedial volumes.

Numerical groundwater models can be used to develop remedial guidelines for groundwater-mediated exposure pathways that are based much more closely on the actual contaminant distribution at a site, and thus avoid the overestimation of contaminant mass inevitably associated with the application of Tier 1 and Tier 2 guidelines. Remedial approaches based on numerical groundwater models use an estimate of the actual residual contaminant mass in a system after remediation is complete and are a key tool in developing viable remedial plans at large and complex contaminated sites.

This approach has been used successfully at a selection of sites in Alberta and elsewhere over the past few years. This report summarizes some of the successful approaches that have been used in Alberta and elsewhere and suggests a best management practice for developing remedial action plans (RAPs) based on numerical modelling approaches.

This report is written in the context of the Alberta Contaminated Sites Framework. However, much of the content of this report has applicability in and can potentially be adapted to a range of regulatory jurisdictions.

For the purposes of this document the term “Numerical Model Approach” refers to a remedial strategy determined from a numerical groundwater model.

1.1 Objective

The overall objective of this report is to develop guidance for best management practices for remedial action plans based on numerical modelling approaches.

1.2 Acknowledgements

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2.0 PROBLEM STATEMENT AND CONTEXT

This project proposes best management practices for developing remedial action plans that are based on numerical modelling approaches. Key aspects of these approaches are expanded in the following sections.

2.1 Limitations of Conventional Approaches

Conventional approaches to management and closure of contaminated sites typically involve assessing contaminant concentrations in soil and groundwater to Tier 1 or Tier 2 soil or groundwater remediation guidelines. These approaches consider and calculate guidelines for a range of exposure pathways including groundwater mediated pathways. Depending on the chemicals of potential

concern (COPCs) and other site conditions, the limiting guideline that “drives” remediation can be the guideline calculated for a range of different exposure pathways.

Exposure pathways that commonly generate limiting guidelines include:

- human direct soil contact;
- human vapour inhalation;
- protection of domestic use aquifer;
- ecological direct soil contact;
- protection of freshwater aquatic life;
- protection of livestock watering; and
- management limit.

Detailed information on all these exposure pathways is available in the Alberta Tier 1 Guidelines document (AEP, 2019a). Of these exposure pathways, only the protection of domestic use aquifer (DUA), the protection of freshwater aquatic life, and protection of livestock watering exposure pathways are mediated by groundwater. The guideline calculations for these pathways depend on a range of parameters including the length, width, and depth of the contaminant “source” area. The guideline calculations for the other exposure pathways noted above do not depend on the size of the source.

The approach developed in this report is only applicable when the limiting guideline at a site is one of the groundwater-mediated exposure pathways and has no relevance in situations where the guidelines for other exposure pathways are limiting.

The conventional approach to Tier 1 or Tier 2 guideline-based remediation planning for a situation where a groundwater-mediated guideline is limiting involves calculating a soil or groundwater remediation guideline based on a set of parameter values that include the source dimensions. The guideline value calculated is the maximum concentration of a chemical within the source volume that will not result in the concentration of that chemical at the exposure point (a Domestic Use Aquifer, a surface water body supporting aquatic life, or a dugout supporting livestock watering) exceeding a threshold value (a drinking water guideline, a surface water guideline protective of freshwater aquatic life, or a livestock watering guideline). It is implicit in these simple models that the source concentration is constant throughout the source volume.

Thus, a conventional numerical guideline is calculated based on the assumption that the residual contaminant mass remaining after remediation is equal to the remediation guideline over the whole source volume (source width x source length x source depth). Case studies have shown that this

assumed contaminant mass can be 1 to 2 orders of magnitude greater than the actual contaminant mass, and this illustrates the degree to which numerical guideline-based remediation can be significantly over-conservative in some cases.

This limitation is typically most significant at larger sites with a complex plume geometry where a groundwater-mediated exposure pathway is the driver for remediation.

2.2 Overview of Numerical Model Approaches

The Numerical Model Approach differs from the conventional remedial guideline approach in that it takes as its starting point the actual (or a best estimate of the) 3-dimensional distribution of contaminant concentrations and predicts how this 3-D plume will move over time. Exposure point locations (typically a domestic use aquifer, a surface water body or a dugout) are identified and the maximum predicted future concentration of the contaminant at the exposure location is predicted. If the maximum predicted future concentration at the exposure location exceeds the applicable regulatory threshold (drinking water, surface water or livestock watering guideline) then that represents a potential risk situation and remedial action is required. The appropriate remedial action is determined through a process of sequential hotspot removal in the numerical model. Blocks of contaminant mass ("hotspots") are removed from the model and the model is re-run. This process is repeated until the maximum predicted future concentration at the exposure point no longer exceeds the regulatory threshold, and the remedial plan for the site is then based on physical removal of the hotspots identified in this process.

The Numerical Model Approach does not generate a unique remedial solution, but rather allows flexibility in removing sufficient contaminant mass to achieve overall remedial goals of no adverse effects to receptors. For example, the remedial planner may wish to balance the relative merits of removing a larger volume of moderately contaminated shallower soil with a smaller volume of deeper soil with a higher chemical concentration. Or there may be scope to compensate for being unable to excavate contaminated material beneath active infrastructure by a larger excavation in accessible areas. Regardless of the remedial plan selected, the Numerical Model Approach allows a proponent to achieve the legislated remedial endpoints of avoiding adverse effects in a way that may provide a viable solution at a complex site where no viable solution might otherwise be available.

Based on the above description of Numerical Model Approaches, it is clear that they require models that are able to take the existing distribution of contaminant in the environment and predict the movement of the associated contaminant plume into the future. This implies the need for a 2- or 3-dimensional numerical model. Model codes are discussed in Section 4.

2.3 Environmental Protection and Enhancement Act (EPEA)

The management of contaminated sites in Alberta is governed under the *Environmental Protection and Enhancement Act* (EPEA; Government of Alberta, 2017). Under EPEA, the primary responsibility of a “Responsible Person” in regard to a contaminated site is to avoid “adverse effect” or to remedy any adverse effects that have occurred.

Numerical Model Approaches are directly focused on developing remedial plans that avoid adverse effect. Thus, Numerical Model Approaches are consistent with the requirements of EPEA.

2.4 Sites at Which a Numerical Model Approach May be Helpful

There are three main indicators that suggest cases where a Numerical Model Approach may be helpful: sites where a groundwater pathway is the driver for remediation; sites with contaminants that are soluble and non-degrading and sites with a greater size and complexity of contaminant plume.

2.4.1 Groundwater Pathways Driving Remediation

Tier 1 and 2 guidelines are typically calculated for a range of exposure pathways (see Section 2.1). The lowest guideline for an applicable exposure pathway is the overall applicable guideline and the corresponding exposure pathway is said to be “limiting” or to be “driving” remediation.

Numerical Model Approaches only have relevance in cases where groundwater-mediated pathways are limiting. When other exposure pathways are limiting, other tools should be employed to develop appropriate remedial plans.

2.4.2 Contaminant Type

The examples of successful application in Section 3 are for chemicals that are soluble and that do not (or are assumed not to) degrade in the subsurface, including chloride, sulphate, and sulfolane. It is anticipated that Numerical Model Approaches will generally be most useful with these types of chemicals. The use of the approach with less soluble chemicals and chemicals that do degrade in the sub-surface is not precluded, but other tools are available that will often help resolve issues with less soluble and degrading contaminants at a lower effort level than attempting a Numerical Model Approach.

2.4.3 Size and Complexity of Plume

In theory, a Numerical Model Approach could be applied to a contaminant plume of any size and complexity. However, the level of effort required to achieve sufficient site characterization to support a Numerical Model Approach will be greater than for conventional approaches. For this reason, a

Numerical Model Approach will generally not be the most efficient solution for relatively small and simple sites. However, as the size and complexity of contaminant issues increase, the effort level involved in the greater site characterization requirements is increasingly offset by a decreased remedial volume and therefore Numerical Model Approaches become increasingly appealing at these larger scales.

2.5 Standardizing Numerical Model Approaches

Developing remedial action plans based on Numerical Model Approaches is a relatively new strategy in Alberta. Having best management practice guidance for such sites will help standardize approaches and assumptions across the industry and may support the development of high-quality reports.

3.0 BACKGROUND INFORMATION

3.1 Examples of Numerical Model Approaches Used for Regulatory Closure

Numerical Model Approaches have been used as a basis for regulatory closure for a range of sites in Alberta and other jurisdictions. Some examples are provided in Appendix A.

3.2 Regulatory Guidance on Numerical Modelling

Guidance on constructing and running numerical models is available from a number of regulatory agencies in Canada, the United States and elsewhere. A summary of some of the more relevant guidance documentation is provide in Appendix B.

4.0 NUMERICAL MODELLING BASICS

4.1 Introduction to Numerical Groundwater Flow and Transport Modelling

Numerical groundwater flow and transport modelling, abbreviated in this document for convenience as “numerical modelling” is a process than can be used to predict the future movement (“transport”) of contaminants in the subsurface. A numerical model consists of a matrix of cells each of which is associated with several hydraulic properties and values for hydraulic head and chemical solute concentration. A simple set of “rules” governs how the values of hydraulic head and chemical solute concentration in one cell affect those in neighboring cells. These “rules” are based on the fundamental equations governing groundwater flow and solute transport, such as Darcy’s law, and standard equations governing diffusion and dispersion of solutes. When the numerical model is “run”, a large set of calculations is made to make sure that the “rules” are met for all pairs of adjacent cells. In this way, the model can apply the fundamental equations of groundwater flow and transport across a 3-dimensional model volume.

4.2 Glossary of Modelling Terms Used in this Report

Numerical groundwater modelling uses several terms that may not be familiar to the general reader. Definitions of some of the more common terms are provided below.

- Boundary Condition – the set of rules that is applied to determine what happens to water and solutes at the Model Boundary. For example, whether the hydraulic head is fixed at the boundary or free to move, and whether water can flow across the boundary.
- GUI – Graphical User Interface (the window on a computer through which a user interacts with a Numerical Model code).
- Model Boundary – any of the edges of the Model Domain including top and bottom.
- Model Cell – the unit used to build up a Model Domain. Each cell has a set of hydraulic properties attached to it including lateral and vertical permeability and porosity, and the Model Code will calculate the values of hydraulic head and solute concentration for each Timestep over which the model is run.
- Model Code – the software package used to set up and run a Numerical Model.
- Model Domain – the 3-dimensional volume in which the Numerical Model is set up and run.
- Numerical Model – a 1-, 2-, or 3-dimensional domain of Model Cells set up to represent and predict groundwater flow and contaminant transport in a corresponding real-world setting.
- Solute Transport – the process by which chemicals dissolved in groundwater travel through the Model Domain.
- Timestep – Models are run over a specified time interval that is divided into Timesteps. Model output values are calculated for each Timestep in each Model Cell.

4.3 Types of Model and Other Considerations

Groundwater flow and transport models can be categorized based on the following considerations (adapted from: Australian Government National Water Commission, 2012):

- Flow dimension: 1D, 2D or 3D. Most model codes can accommodate 3D modelling. However, 3-D modelling is relatively resource intensive and time-consuming. Depending on the complexity of the problem, it may be that a 1-D or 2-D model can provide an adequate solution without resorting to a full 3D model.
- Model type: analytical *vs* numerical. This document is primarily focussed on approaches using numerical models. Numerical models involve setting up a grid of cells throughout a model domain and solving equations for each pair of adjacent cells or nodes, as summarized in Section 6.1 above. The conventional equations used to calculate Tier 1 and Tier 2

groundwater guidelines are examples of analytical models where equations are used to solve flow and transport problems without setting up a grid of cells.

- Model type: finite element *vs* finite difference. These two model types use fundamentally different ways of setting up and linking a domain of cells. Both are equally acceptable for the purposes of this document, and the differences between them, though important to modellers, are not significant for the purposes of this document.
- Saturated *vs* un-saturated flow. Most models are primarily set up to handle either saturated flow (below the water table) or unsaturated flow (above the water table). Some models have a limited capacity to handle both flow types. For problems that are primarily in the vadose zone it is optimal to choose a model that is primarily designed for unsaturated flow. For problems that are primarily below the water table, it is best to select a saturated flow groundwater model.
- Porous medium *vs.* fracture flow. Most numerical models used in the management of contaminated sites assume that the standard equations controlling flow through a porous medium are applicable. Models where flow is primarily through a network of fractures are more complex and sufficient data to support such models is rarely available in contaminated site management scenarios.
- Steady-state *vs* transient models. Transient models calculate how hydraulic head and solute concentrations vary over time throughout the model domain. Steady state models reflect only the final, steady state achieved in a model when sufficient time has passed for the model to have finished responding to changes in inputs. For practical purposes, many numerical models developed to help manage contaminated sites use a steady state flow model and a transient solute transport model.
- Solute transport capabilities. Most models developed to help manage contaminated sites include advective transport as well as the processes of diffusion, sorption and decay.

It is preferable to select a model code that is well documented, has previously been verified and is widely used and accepted by the modelling community (a group of such codes is provided in Table 1). If an existing verified code is selected but is modified or altered for the purpose of a modelling exercise, or if a newly developed code is chosen for a study, it is recommended that a section demonstrating the accuracy of its simulation capabilities be included in the report (CEMA, 2012).

4.4 Numerical Model Codes

As indicated in Section 5.2, the term “numerical model code” refers to the software package used to set up and run a numerical model. The model code can be considered as the “platform” that implements the fundamental equations of groundwater flow and transport across a 3-dimensional

space. Most numerical models have at their core a very similar set of fundamental equations to calculate flow and transport.

A wide variety of numerical model codes are in use. Table 1 provides a summary of some of the more commonly used numerical model codes current in Canada and elsewhere. This list is not exclusive and is not intended to preclude the use of any other numerical model code that can be shown to be valid.

Table 1 Modelling Codes Commonly Used in Canada		
Model Code	Type	Overview
MODFLOW*	Saturated Flow	Free public-domain source code using modular finite-difference to solve the groundwater flow equation.
MODFLOW-SURFACT	Saturated and Unsaturated Flow; Solute transport	Commercial software developed specifically to overcome limitations associated with MODFLOW and MT3D.
FEFLOW	Saturated and Unsaturated Flow; Transport of Mass and Heat; Integrated GUI	Commercial software using finite element analysis to solve the groundwater flow equation for both saturated and unsaturated conditions as well as mass and heat transport, including fluid density effects and chemical kinetics for multi-component reaction systems. Software has an integrated GUI.
HYDRUS (2D and 3D)	Unsaturated and Saturated Flow; Transport of Heat and Multiple Solutes	Commercial software using finite element analysis to solve the groundwater flow equation. The primary design function of this software was to solve unsaturated flow problems, but it is also capable of working for both saturated conditions as well as mass and heat transport. Software has an integrated GUI.
HydroGeoSphere (HGS)	Saturated and Unsaturated Flow; Transport of Mass and Heat	Commercial software based on a 3D control-volume finite element groundwater model. Can take into account all key components of the hydrologic cycle, including terrestrial components.
MT3D/MT3DMS	Transport of single or multiple reactive solutes in GW	Open source software developed to compute coupled flow and transport when coupled with MODFLOW.
RT3D	Multi-species Reactive Transport in GW	Open source software developed to compute coupled flow and transport when coupled with MODFLOW.

Table 1 Modelling Codes Commonly Used in Canada		
Model Code	Type	Overview
PHT3D	Multi-species Reactive Transport in GW	Open source software developed to compute coupled flow and transport when coupled with MODFLOW. Includes MT3DMS and PHREEQC.
SEAWAT	Saturated Flow and Transport of Multiple Solutes and Heat	Open source software combining MT3DMS and MODFLOW to simulate density-coupled flow and transport.
Hydrological Simulation Program – FORTRAN (HSPF)	Integrated watershed hydrology model	Free public domain source code used to simulate natural and anthropogenic hydrologic processes.
ZONEBUDGET	Add-on for Mass Balance Calculation in MODFLOW	Open source software generally integrated with MODFLOW GUIs.
MODPATH	Add-on for Particle Tracking in MODFLOW	Open source software generally integrated with MODFLOW GUIs.
UCODE	Add-on for Parameter Estimation and Uncertainty Analysis	Open source software compatible with any model and allowing for parameter estimation and sensitivity analysis.
PEST	Add-on for Parameter Estimation and Uncertainty Analysis	Open source software compatible with any model and allowing for parameter estimation and sensitivity analysis. Available with compatible versions for many model and GUIs.
MIKE 11/ MIKE SHE	Surface water modelling	Commercial software to model flow in network of rivers and streams. Has an integrated GUI and can be coupled with MODFLOW.
GS-Flow	Coupled surface water-groundwater	Public domain code coupling existing surface water model (PRMS) with MODFLOW.
Visual MODFLOW and Visual MODFLOW Flex	GUI	Commercial graphical user interface (GUI) for MODFLOW and MODFLOW add-on
Groundwater Vistas	GUI	Commercial graphical user interface (GUI) for MODFLOW and MODFLOW add-on
GMS	GUI	Commercial graphical user interface (GUI) for MODFLOW and MODFLOW add-on

* MODFLOW-96, MODFLOW-2000, MODFLOW-2005, MODFLOW-OWHM, MODFLOW 6

5.0 REQUIREMENTS FOR AN ACCEPTABLE NUMERICAL MODEL

As indicated in Section 4, there is a large body of regulatory guidance documents that provide detailed input into every aspect of the process of planning and building a numerical groundwater model. As summarized in Section 4.3, there is significant consistency in what is considered best practice in numerical modelling across regulatory jurisdictions in various parts of the world, as well as across models built for different purposes (contaminated site management, water resource management or environmental impact assessment).

It is not the purpose of this document to act as a primer on how to construct a numerical groundwater model, and accordingly the excellent guidance available elsewhere is only summarized here to provide context to the modelling process.

5.1 Overview

Typically, the steps involved in developing a numerical groundwater model should include, at minimum, the following:

- development of a Conceptual Site Model;
- selection of an appropriate mathematical model and code;
- model set-up;
- groundwater flow calibration and verification;
- transport model selection, predictions and verification; and
- uncertainty assessment/ sensitivity analysis.

A summary of each of these steps is provided in the following Sections.

5.2 Conceptual Site Model

The first step in constructing an acceptable model is the development of a conceptual site model (CSM). A CSM to support the development of a numerical model is generally similar to the CSM required in “conventional” contaminated site management. The CSM required to support a numerical model includes of a set of assumptions describing the groundwater system and transport mechanisms (Bear *et al.*, 1992). The assumptions should be specific to the site or problem to be modelled and should include information such as the geometry, lateral and vertical length and thicknesses, geology of the different layers and their hydrogeological properties (hydraulic conductivity, porosity, storativity, anisotropy, *etc.*), flow regime, boundaries (recharge and discharge areas), initial conditions (groundwater contour map), *etc.*

The overall modelling objective and the problem to be solved must be clearly formulated. An appropriate numerical model cannot be constructed if the modeller does not have a good understanding of the system, the problem to be simulated and the modelling objective. For Numerical Model Approaches the problem to be solved will normally be predictions of maximum future contaminant concentrations at clearly specified exposure points, such as the maximally affected location within a DUA, or the location of groundwater discharge to a surface water body or dugout. The overall modelling objective will normally be identifying the remedial actions that will ensure regulatory thresholds are not exceeded at identified exposure points.

It is important to assess the proper degree of complexity required for the CSM and ultimately of the numerical model. An oversimplified CSM and model may lack some of the required information essential to reproduce the system appropriately; an over complicated CSM and model may be impractical, time consuming and costly, and furthermore may lack data required to calibrate and verify the model (Bear *et al.*, 1992). The appropriate degree of complexity of the CSM and accuracy required for the model should be carefully assessed based on the objective of the modelling exercise, available resources, available data and regulatory framework in which the model output will be evaluated.

In the context of the Numerical Model Approaches for risk-based site closure discussed in this document, the CSM should include, at a minimum, the following elements:

- A summary of the site setting, including as a minimum information on location, historical operation, historical spill information, topography, land use, and nearby surface water features.
- Identification of geological and hydrogeological units including stratigraphy/texture, hydraulic properties and spatial extent of each unit.
- Identification of Chemicals of Potential Concern (COPC) with rationale, identification of chemicals to be modelled with rationale, and 3-dimensional distribution of chemicals to be modelled.
- Identification of applicable exposure pathways and associated receptors, inducing an indication of which exposure pathway(s) are limiting for the various COPC.

5.3 Model Code Selection

This step consists in selecting an appropriate numerical model code. One key consideration in this process is to understand whether the problem to be solved is primarily in the unsaturated or saturated zone and then to select a model which will handle the situation effectively. Many of the available codes are summarized in Table 1, and there is a large amount of information on model code selection available in the references in Section 4.

5.4 Model Domain and Boundary Conditions

This step involves setting up the spatial framework within which the model will be run. Important choices to be made include the spatial dimensions of the domain and the cell size. The domain should be large enough in all dimensions to accommodate the current plume, the receptor locations to be modelled, and have boundaries far enough from critical model areas so as not to perturb the results at key model locations.

The default assumption is perhaps that numerical groundwater models are built in 3 dimensions. However, there are occasions where the essence of a problem can be represented by simply modelling one or more 2-dimensional “slices” through the area of interest, and this may turn out to be a more efficient solution in some cases.

The model boundary conditions are the rules that are applied to the edges of the model domain that govern what happens to hydraulic head and water flux at those edges. There is plenty of guidance on this aspect available in the source material referenced in Section 4.

All numerical models must start from a specified set of initial conditions that define the starting hydraulic head in each cell, among other things. Selecting a set of initial conditions that is relatively realistic will tend to result in a model that converges more efficiently, but the initial conditions do not affect the final outcome of the model so long as they do not drive the model into instability.

5.5 Groundwater Flow Calibration and Verification

All numerical groundwater flow models need to be calibrated prior to being used for prediction. Calibration involves refining the initial estimates (layer/aquifer properties and boundary conditions) until the model satisfactorily reproduces the real-world system. Calibrating a flow model involves comparing a set of model outputs with the corresponding set of calibration targets measured in the real world. For practical purposes, the calibration targets typically used in Numerical Model Approaches are either a set of hydraulic heads measured in a group of monitoring wells, or a set of groundwater head contours (lateral and vertical) interpreted between hydraulic head measurements at monitoring wells. Key model input parameters such as the hydraulic conductivity and porosity of each layer, surface infiltration rate and boundary conditions are adjusted to try and improve the fit of predicted to actual hydraulic heads. This needs to be done not only laterally, but also vertically throughout the model domain.

Flow calibration can be conducted in steady-state or in transient state. Steady-state is the most commonly used method because i) sufficient data for a transient flow calibration are typically not available, and ii) the steady-state flow field is adequate for modelling longer-term contaminant

transport. Calibration can be conducted manually or using a parameter-estimation tool (such as PEST or UCODE, see Table 1).

Once a satisfactory calibration between model prediction and field data has been achieved, a few crucial points need to be checked to verify the reliability of the prediction, namely the convergence criteria and the model mass balance (as applicable – mass balance may not be readily available for finite-element models).

The goodness of a calibration can be assessed by comparing predicted *versus* field values and calculating the mean error, mean absolute error, root mean square error, standard error, and most importantly by using common sense. Model residuals (*i.e.*, difference between predicted *versus* observed) are unavoidable because all numerical models are necessarily a simplification of real-world conditions. The acceptable percentage of error or residual is site-specific, but the values should be presented, and a rationale provided to explain why the numbers are reasonable for the model.

5.6 Transport Model

Groundwater transport modelling should not be initiated until a reasonable calibration of the groundwater flow has been achieved. In some instances, running transport scenarios may trigger a re-evaluation of the calibrated flow model. All numerical groundwater flow models are subject to non-uniqueness in solution, *i.e.*, different sets of parameters and boundary conditions can result in similarly calibrated models. By adding another level of complexity with the contaminant transport, the flow calibration selected may need to be challenged and re-assessed.

Modelling of solute transport is challenging, often more so than modelling groundwater flow, for several reasons. For one, it is more difficult to characterize the contaminant plume and transport mechanisms. Often the source location, concentration and timing of release is unknown. The transport mechanisms involved, and potential natural attenuation mechanisms are also often imperfectly understood resulting in a larger number of assumptions required to model solute transport. Secondly, the governing equations do not always completely represent what is observed in the field (Konikow, 2011). Effective solute-transport modeling may be achieved by keeping the model relatively simple and by using it to test and improve conceptual understanding of the system and the problem to be solved. It should not be expected that all concentrations observed in the field can be reproduced accurately in the model (Konikow, 2011).

In an ideal world, the transport model would be calibrated by inputting the timing, extent and composition of historical contaminant releases and re-creating a rough approximation of the current plume distribution. There may be contaminated sites where source information is sufficiently detailed that this process is feasible and useful. However, in practice, for most real-world contaminated site problems, relevant details of historical releases may be vague or non-existent. In

these cases, strict transport model calibration will not be possible, but it should still be possible to use the transport calibration mechanism to demonstrate that the current plume could plausibly have resulted within known or assumed constraints on source timing, extent and composition. While not a formal transport calibration, this process still provides a practical reality check on the transport parameters in the model.

The steps involved in running the transport model in a Numerical Model Approach are as follows:

- Start with a calibrated flow model (normally steady state).
- Use known or assumed constraints on source timing, extent and composition to provide a reality check on the transport parameters in the model. If detailed information on historical sources is available, it may be possible to conduct a more formal transport model calibration.
- With the calibrated model, input the current 3-dimensional distribution of the chemical to be modelled.
- Run the model and generate predicted chemical concentrations as a function of time at the selected exposure points in the model.

5.7 Uncertainty, Sensitivity Analysis and Conservatism

There is uncertainty inherent in any predictions of contaminant concentrations in the subsurface. This is due to a range of factors including the heterogeneity of subsurface materials and the simplifications inevitably involved in representing 3-dimensional contaminant distributions based on a limited number of discrete measurement points.

Sensitivity analysis can be an appropriate technique for assessing model uncertainty. Model sensitivity analysis should be conducted on calibrated models and when running predictions, to assess parameters that are the most sensitive and assess the degree of uncertainty that exists in the predictions. Sensitivity analysis consists in varying one or more of the model parameters or boundary conditions and comparing the output to the base calibrated model or base prediction. Sensitivity analysis can be conducted manually or using an automated tool such as PEST or UCODE.

The objective is to quantify the response of the model output (hydraulic head, flux or mass) to an incremental variation in model inputs. Parameters that affect the calibrated results but do not affect the model predictions are not a concern. Parameters that affect the calibration but do not affect the prediction are a concern but can be resolved by rigorous calibration. Parameters that do not affect calibration but do affect the prediction results are the most concerning as they are related to model non-uniqueness. These parameters should be strictly based on site specific data and not estimated during model calibration due to the influence they have on the model predictions.

The results of the sensitivity analysis can be used to generate a realistic range of possible model outputs. The model output carried forward to develop the remedial plan should be towards the conservative end of the range of possible outputs, such that a worse outcome than predicted by the model is unlikely. Rationale should be provided as to why the model output carried forward to the remedial plan is suitably conservative.

5.8 Model Reporting and Output

Model reporting should summarize the conceptual site model and provide a succinct summary of salient elements of how the model was built and the rationale for doing so. Flow model initial input parameters should be tabulated together with the post-calibration input parameters for comparison. Rationale should be provided confirming that the calibrated parameter values are within reasonable ranges for the stratigraphic units and site conditions described in the CSM. The flow model calibration process should be described, and the criteria for the acceptability of the final calibration should be clearly stated with rationale.

The report should describe the extent to which it was possible to achieve transport model calibration and/or the extent to which it was possible to provide a reality check on the transport parameters in the model consistent with the comments in Section 5.6 above. Transport model output should normally be provided as a graphical output showing predicted concentration *vs* time at appropriate receptor point locations. The relevant threshold (drinking water guideline, surface water guideline *etc.*) should be clearly indicated on the graphs.

6.0 APPLICATION OF NUMERICAL MODEL TO DEVELOP REMEDIAL PLAN

Section 5 described a fairly standard process to develop a numerical groundwater model to predict maximum future contaminant concentrations at exposure points such as an underlying domestic use aquifer, a surface water body, or an actual or potential livestock watering dugout. Section 5 ended at the point where the model had predicted how the concentration of the chemical being modelled would be expected to vary over time at the exposure point(s).

If the predicted concentrations at the exposure point(s) never exceed the relevant threshold values, then the model provides support for bringing the site to closure without any further remediation in relation to the COPC(s) and exposure pathway(s) modelled. If, however, COPC concentrations at the exposure points are predicted to exceed the relevant threshold values at some point, then the next step is to use the model to develop a numerical model-based remedial action plan for the site. The remainder of Section 6 describes this process.

6.1 Demonstrating Conservatism

At Tier 1 and Tier 2, uncertainty in model output is managed by using reasonable worst-case values of key input parameters such that there can be confidence that a worse outcome than predicted by the model is unlikely.

The corresponding process for a remedial plan based on numerical modelling is sensitivity analysis. As indicated in Section 5.7, it is important that sensitivity analysis be carried out on the numerical model, that the model output carried forward to the remedial plan is sufficiently conservative that a worse outcome than predicted by the model is unlikely, and that suitable rationale is provided supporting this.

6.2 Hotspot Removal to Achieve Exposure Point Compliance

The groundwater flow and transport model created in Section 5 can be used to generate a numerical model based remedial action plan for the site simply by removing parts of the source area in the model until the predicted concentrations of the COPC(s) modelled never exceed the relevant threshold values at the exposure point(s). Typically, this is done iteratively, by removing blocks of contamination from the model and re-running until the predicted exposure point concentrations no longer exceed their respective thresholds. The blocks of contaminant removed from the model then define the areas of the site that require remediation.

This process does not create a single, unique remedial solution, but rather allows the modeller/remedial planner to make value judgements about which parts of the source area offer the most effective path to meeting remedial goals. Typically, this will be the areas with the highest concentration (“hotspots”) with consideration for the fact that shallower material may be easier to access than deeper material.

Once the remedial plan is generating a compliant solution in the model, the remedial planning process can proceed.

6.3 Other COPC and Exposure Pathways

Sites that proceed to risk-based closure using a Numerical Model Approach often have one primary contaminant with remediation being driven *via* one or more groundwater-mediated exposure pathways. The modelling process described in Sections 5 and the previous parts of Section 6 helps develop a risk-based remedial plan to resolve issues related to that contaminant and those exposure pathways. However, remediation planning also needs to make sure that remediating the primary COPC(s) also achieves appropriate remedial goals for all other COPCs that may have been identified for the site considering not only groundwater-mediated exposure pathways but all other remedial pathways as well.

6.4 Updating Model in Remedial Phase

Sufficient delineation of contaminant distribution(s) is required prior to starting the modelling process to enable a risk-based remedial plan to be developed for a site. However, additional contaminant distribution data is often collected as the remedial activities proceed, either because some previously inaccessible areas are now available for sampling, and/or from confirmatory samples collected from the base and walls of the excavation(s).

If the contaminant concentrations measured during the remedial phase differ dramatically from the concentrations assumed in the model, it may be worthwhile re-running the model with an updated contaminant distribution to check whether any updates to the remedial plan are required. Typically, the incremental level of effort to make these model updates will be small in relation to the total effort required to build the model, and there is a clear advantage in knowing what changes are required to the remedial plan while equipment is still on site. Regardless, once remediation is complete, all available confirmatory and other data should be used to update the model and confirm that an acceptable remediation plan has been completed. This will provide validation that the remediation is complete.

7.0 BEST MANAGEMENT PRACTICES FOR NUMERICAL MODEL APPROACHES

The overall purpose of this document is to provide the context and technical backing for the recommended best management practices for Numerical Model Approaches in this Section. The best management practices in this section are intended to provide guidance to proponents developing remedial action plans based on Numerical Model Approaches, and also to provide some reference points for those reviewing such approaches. Modelling review is an essential but difficult task as the reviewer needs to clearly understand the strengths and limitations of the model without having to reproduce the entire analysis (USGS, 2004). Additional information on model review is available in USGS (2004) and BC MoE (2012).

The bullet points in Sections 7.1 to 7.5 below indicate specific elements of the numerical model and the associated remedial action plan that should be present in a well-crafted Numerical Model Approach. The elements listed below can be validated without needing to re-create the numerical model and thus can serve both as a checklist to a proponent building such an approach, and also provide reference points for model review.

Some of the bullet points are quite prescriptive, while others call for some level of professional judgement. For issues that are judgement based, the appropriate criterion to apply is whether the element in question has been achieved sufficiently to provide a reasonable level of confidence in the conclusion that conducting the proposed remedial program will prevent the risk of receptors experiencing adverse effects in the future.

7.1 Overall Model Objective and Modelling Problem to be Solved

The first step in developing a remedial action plan based on a Numerical Model Approach is to check that the objective of the study is clearly specified. Only if the objective is clearly stated can the adequacy of the model be evaluated (USGS, 2004). Two critical elements need to be clearly understood and stated: the overall model objective and the modelling problem to be solved.

Typically, the overall model objective will be to develop a Remedial Plan based on a Numerical Model Approach that will protect all appropriate receptors from current and potential future adverse effects.

The modelling problem to be solved will typically be to predict future concentrations of modelled chemicals at specified receptor locations to allow the Numerical Model Approach to be developed. The selection of chemical(s) to be modelled and receptor locations to be assessed must be clearly justified.

7.2 Appropriateness of Numerical Model Approach

The appropriateness of using a Numerical Model Approach at the site should be clearly justified. Section 2.4 of this report indicated some suggested conditions where a Numerical Model Approach is more likely to be helpful. These conditions are:

- Groundwater pathways drive remediation.
 - The Numerical Model Approach described in this document has no applicability unless the limiting exposure pathway driving remediation is groundwater mediated.
- Contaminant(s) driving remediation are soluble and non-degrading.
 - For contaminants that degrade in the sub-surface, typically other tools will provide a more streamlined path to closure.
- The plume is sufficiently large and complex to require this approach.
 - Smaller and simpler sites will normally be managed more efficiently using other techniques

The intention of this section is not necessarily to exclude sites that do not meet all these conditions, but at least to require justification for why the Numerical Model Approach is required at a particular site.

7.3 Conceptual Site Model

The conceptual site model (CSM) should include enough information to support the building of a credible numerical model and the associated remedial action plan. Additional material that does not relate to these needs is not helpful and detract from the clarity of the report.

The required site characterization detail is higher than would be typical for a site assessed under conventional Tier 1 or Tier 2 guidelines. In order to build a 3-D model that will adequately represent ongoing contaminant transport it is necessary to understand the disposition of the major stratigraphic layers that will affect transport and to characterize the contaminant distribution in 3-dimensions. An adequate level of site characterization needs to be assessed in the context of what is reasonable to achieve on a commercial site that is not a research facility. Increased delineation is always possible, but the appropriate assessment standard is whether delineation is sufficient to provide confidence that a remedial action plan based on a Numerical Model Approach will adequately protect receptors from current or future adverse effects.

Required CSM components are discussed in the following sections.

7.3.1 Site Setting

Summary information on site setting will be helpful to understand the context of the site. Relevant information includes site operational history including timelines and any available information on historical spills. This will help confirm that the chemicals of potential concern and the selections of chemical(s) to be modelled (Section 7.3.3) are appropriate. Summary information on topography and nearby surface water bodies will help understand whether the appropriate exposure pathways have been considered (Section 7.3.4).

7.3.2 Geological and Hydrogeological Units

- The CSM should clearly identify the number and character of units present.

Typically, the appropriate number of units will be the minimum number that adequately describe the flow regime. For example, the change from a fine-grained unit to a coarse-grained unit will normally be significant, while the difference between two different fine-grained units may not be. Continuous coarse-grained layers should be modelled, but isolated lenses of coarse material can often be considered part of the fine-grained layer they reside in.

- Unit properties should be clearly stated/summarized.
- Rationale for the properties should be provided.
- The hydraulic properties for a unit can be a single value, or a spatial distribution, if rationale and a clear description are provided.

These will form the starting point for model set up.

- Do unit hydraulic properties make sense with the units described?

The properties indicated should be broadly consistent with the stratigraphy of each unit.

7.3.3 Chemicals of Potential Concern and Chemicals to be Modelled

There is an important distinction to be made here between chemicals of potential concern (COPC) and chemicals to be modelled. Chemicals of potential concern are all site-related chemicals that exceed appropriate screening guidelines. Typically, it will be necessary to model only a subset of the COPCs, and often only a single chemical needs to be modelled to develop an appropriate risk-based remedial plan. An example might be a site with F2 and F3 hydrocarbons exceeding screening guidelines in soil, and sodium and chloride exceeding screening guidelines in groundwater. They are all COPC, but only the chloride is modelled, since hydrocarbon remediation (in this case) is not driven by groundwater pathways, and the sodium and chloride are associated, so that a remedial plan to manage chloride will also manage the sodium.

- Are the COPC(s) clearly identified with screening rationale provided?
- Are sufficient data provided to confirm that other potential site-related chemicals are not COPCs?
- Are the chemical(s) to be modelled clearly identified with rationale provided?
- Is the distribution of chemical(s) to be modelled adequately characterized in 3-dimensions to support building a transport model?

7.3.4 Exposure Pathways and Associated Receptors

- Are the applicable exposure pathways and associated receptors identified for the COPCs noted above?
- Is the limiting pathway for the COPC(s) to be modelled clearly identified?
 - Is it a groundwater pathway?
 - Are there other relevant groundwater pathways that can/should also be assessed in the model (*e.g.*, protection of DUA, protection of freshwater aquatic life, protection of livestock watering *via* dugout)?

7.4 Validity of Numerical Model

This section highlights specific elements that can be assessed to help assesses the validity of the numerical model without independently re-creating the model.

7.4.1 Model Domain and Cell Size

This section assesses the model domain, which is a 3-dimensional gridded volume made up of model cells.

- Is the lateral extent of the model domain appropriate?

The model domain should extend upgradient, downgradient and laterally of the plume of modelled contaminant(s) sufficiently to show unimpacted areas on all sides. Additionally, it needs to extend sufficiently to include any surface water receptor locations or discharge points such as ponds, creeks or dugouts that are being modelled.

- Is the vertical extent of the model domain appropriate?

The model domain needs to extend vertically at least far enough to include the actual or assumed DUA beneath the site if the DUA pathway is being modelled, and far enough that the boundary condition at the base of the model doesn't result in any perturbation of the modelled flow field at the top of the DUA.

- Is a rationale for the cell size provided and appropriate?

Selecting cell size is a compromise between being able to model available detail in contaminant distribution and stratigraphy and having a model that can be run and iterated in an acceptable length of time. Cell size also controls the minimum volume of soil that can be removed from the model when exploring potential remedial scenarios. Using a smaller cell size close to source areas and larger cells in distal areas may be helpful if available in the model code used.

- Does the top row of cells in the DUA have a thickness of 2 m?

The Alberta Tier 1 and 2 model for assessing potential impact to a DUA assumes a minimum screen length of 2 m for a water well. This implies an assumption that water entering a domestic use well has a vertical mixing depth of 2 m. The most appropriate way of simulating this same requirement in a model is for the top layer of cells in the DUA to have a 2 m thickness. This effectively imposes a 2 m mixing zone at the top of the DUA in the model.

7.4.2 Boundary Conditions

- Are the model boundary conditions clearly stated for all model edges, is rationale provided for why these types/values of boundary condition were used and do they make physical sense?

Model boundary conditions are the "rules" about what happens at the edges of the model domain. Typical boundary condition types include constant head boundaries which might be used at the

upgradient and downgradient edges of a simple rectangular model with a relatively uniform, planar flow field. No-flow boundaries might be used at model edges that run approximately parallel to groundwater flow and possibly at the base of the model. A specified flux boundary might be used at the top of the model to represent infiltrating precipitation adding water to the model at the water table. There are no hard and fast rules, but the types and values of boundary conditions should make physical sense to the modeller and to the reviewer in relation to the real-world elements being represented. This check provides a level of confidence that the physical processes in the model are appropriate to the situation being modelled. In practice, if model boundary conditions are inappropriate, it is unlikely that an acceptable model calibration will be achievable (Section 7.4.4).

7.4.3 Hydraulic Properties

- Is a rationale provided for the initial hydraulic properties used in the model and are these clearly tabulated for the following?
 - Lateral hydraulic conductivity for each stratigraphic unit/model layer;
 - Vertical hydraulic conductivity for each stratigraphic unit/model layer;
 - Effective porosity for each stratigraphic unit/model layer; and
 - Infiltration rate at the surface of the model?
- Do the values make sense in relation to the stratigraphic units identified and the site setting?

Note that these properties may change during the process of calibration, but both initial and calibrated values should be within physically reasonable ranges based on the stratigraphy defined and the climatic conditions for the site location.

7.4.4 Flow Model Calibration

A typical workflow for groundwater modelling involves imposing initial values of hydraulic properties (Section 7.4.3) on the model defined by the model domain (Section 7.4.1) and boundary conditions (Section 7.4.2) and then running the model to determine the steady state distribution of hydraulic head (water level and vertical hydraulic gradient). The modelled distribution of hydraulic head is then compared to the measured distribution, and the hydraulic properties and possibly boundary conditions are adjusted to optimize the fit between modelled and measured head.

- Are the calibrated hydraulic properties used in the model clearly tabulated for the following:
 - Lateral hydraulic conductivity for each stratigraphic unit/model layer;
 - Vertical hydraulic conductivity for each stratigraphic unit/model layer;
 - Effective porosity for each stratigraphic unit/model layer; and
 - Infiltration rate at the surface of the model?
- Do the values make sense in relation to the stratigraphic units identified and the site setting?

- Does the calibrated distribution of hydraulic heads across the model domain acceptably reproduce the measured distribution of hydraulic heads:
 - laterally; and
 - vertically?

There are various measures of “goodness of fit” between modelled and measured hydraulic head. These are good tools for modellers to know if one calibration iteration is better or less good than the previous one, and may be of value in the review of a model, but perhaps a more intuitive way to determine whether a model calibration is fit for purpose is a visual comparison of the groundwater contours generated by the model and the measured groundwater contours. This should be done in both plan view and in at least one representative cross section aligned parallel to groundwater flow. A perfect calibration will never be achieved. The assessment criterion should be whether the calibration achieves a reasonable approximation of the measured flow field and therefore whether the remedial action plan based on a Numerical Model Approach is likely to achieve its stated objective.

In summary, if a groundwater calibration has achieved a reasonable approximation of the measured lateral and vertical distribution of hydraulic heads, and the hydraulic properties used to achieve the calibration are broadly consistent with the stratigraphic units identified and the site setting, then the groundwater flow model is fit for purpose.

7.4.5 Transport Model

From a purely theoretical standpoint, the ideal way of setting up a transport model would be to input the locations and magnitude of historical contaminant releases into the flow model, run the flow model forwards to the present day to reproduce the current contaminant distribution, and continue running the model to predict future contaminant distribution. This approach may be feasible in a research aquifer where the input of contaminants can be known and carefully controlled. However, at real world contaminated sites this approach is normally not feasible since the timing, exact location and source composition are typically not known in detail for historical releases.

In lieu of a formal transport model calibration, it may be possible to demonstrate that the current plume could plausibly have resulted based on known or assumed constraints on source timing, extent and composition. While not a formal transport calibration, this process may still provide a practical reality check on the transport parameters in the model.

Often the best available solution will be to superimpose the known, current contaminant distribution on top of a calibrated flow model and allow that to predict the development of the contaminant plume over time. For practical purposes, this is the modelling methodology that will be used to predict future contaminant distributions at most real-world contaminated sites.

The following points should be checked during the review process:

- Is the contaminant distribution input into the model consistent with the current distribution of measured contaminant concentrations?

Typically, this will be best achieved by comparing the model input concentrations with a contoured interpolation of the measured concentration values in plan view and for one or more vertical cross-sections.

- Does the movement of contaminant plumes predicted by the model make sense in general terms based on the measured lateral and vertical hydraulic gradients and stratigraphic units present?

7.4.6 Model Output

- Does the model clearly provide predicted future concentrations of modelled COPC(s) at exposure point locations and indicate maximum predicted future concentrations?
- Are the exposure point locations appropriate?
- Is the maximum projected future concentration at the exposure point locations(s) clearly indicated and compared to applicable threshold/guideline values?

In the case of a surface water body (pond, creek, spring) the model output should represent the actual location of the water body. In the case of a dugout the model output should represent either the actual location of the dugout, and/or the reasonable worst-case location where a dugout could be constructed, depending on the site situation. For a DUA, the model output should represent the worst-case location in the top 2 m of the DUA. The worst-case location will be at the center of the predicted plume viewed at the top of the DUA and at the time of maximum future concentration at the top of the DUA.

7.5 Application of Numerical Model to Develop Remedial Plan

7.5.1 Remedial Plan

In Section 7.4.6, model output was generated for actual or worst-case receptor locations for the status quo scenario without any remediation. Model output showing current or future exceedance of threshold values (drinking water guideline, surface water guideline or livestock watering guideline, as appropriate) indicates the need for remediation. Remediation is modelled by sequentially removing contaminant mass “hotspots” from the model.

- Does the report clearly indicate the extents of the area(s) where remediation is proposed?

- Does the model successfully demonstrate that removing the material indicated will result in no future exceedance of applicable threshold/guideline values at exposure point locations?

7.5.2 Updates to Remedial Plan

Sufficient delineation of contaminant distribution(s) is required prior to developing a remedial action plan for a site. However, additional data is often collected as the remedial activities proceed, either because some previously inaccessible areas are now available for sampling, or from confirmatory samples collected from the base and walls of the excavation(s).

- Is there a plan to re-run the model once remediation is complete accounting for additional chemical concentration data collected during remediation to determine whether any updates to the remediation plan are required to ensure protection goals are met?

7.5.3 Other Chemicals of Potential Concern and Exposure Pathways

This document has focussed on a process to review risk-based remedial plans that are based on numerical modelling for one or a small number of contaminants for which remediation is being driven by groundwater-mediated pathways. However, it is also important to confirm that sufficient remedial measures are being put in place to ensure issues related to any other COPCs identified for the site and for any other relevant exposure pathways are addressed satisfactorily to ensure adverse effects are avoided.

- Are the proposed remedial measures sufficient to address all chemicals of potential concern at the site considering all relevant exposure pathways as well as the chemicals of potential concern that were modelled and the groundwater pathways that they were modelled for?

7.6 Review Summary and Conclusion

If the remedial action plan based on a Numerical Model Approach has adequately demonstrated the points indicated in Section 7, then there is an acceptable level of confidence that the remediation proposed in the Numerical Model Approach based Remedial Plan will achieve receptor protection goals consistent with EPEA requirements.

8.0 CLOSURE

This report was prepared by Millennium EMS Solutions Ltd. ("MEMS") for the Petroleum Technology Alliance of Canada ("PTAC") and has been completed in accordance with the terms of reference in the Recipient Agreement dated May 1, 2018 for PTAC Project reference 18-RRRC-03. This report does not necessarily represent the views or opinions of PTAC or the PTAC members.

While we have made every attempt to ensure that the information contained in this report is complete and has been obtained from reliable sources, neither MEMS nor PTAC are responsible for any errors or omissions, or for the results obtained from the use of the information in this report.

Nothing in this report should be a substitute for independent site investigations and the sound technical and business judgment of the reader. In no event will MEMS, PTAC or their employees or agents, be liable to the reader or anyone else for any decision made or action taken in reliance on the information in this report.

Yours truly,

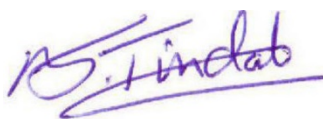
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APPENDIX A: EXAMPLES OF SITE CLOSURE BASED ON NUMERICAL MODEL APPROACHES

Appendix A

Examples of Site Closure Based on Numerical Model Approaches

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This appendix provides examples where Numerical Model Approaches have achieved regulatory acceptance to support risk-based site closure both in Alberta (Section 1) and elsewhere (Section 2).

1.0 ALBERTA EXAMPLES

1.1 Former Sulphur Storage Facility Impacted by Sulphate

Millennium EMS Solutions Ltd. (MEMS) has achieved regulatory acceptance of a remedial action plan based on a Numerical Model Approach for a former sulphur storage and handling facility.

All surface infrastructure and marketable sulphur had been removed from the site and site assessment had been completed at the time the Remedial Action Plan was developed. The primary issues at the site requiring risk management were residual elemental sulphur mixed with soils and dissolved sulphate resulting from *in-situ* oxidation of the elemental sulphur. The elemental sulphur was remediated according to requirements specified in the *Guidelines for Landfill Disposal of Sulphur Waste and Remediation of Sulphur Containing Soils* AENV (2011).

The Conceptual Site Model (CSM) for the site identified a plume of sulphate in groundwater exceeding Tier 1 groundwater guidelines over a large footprint. However, there was a significant vertical separation between the base of sulphate impact, and the shallowest potential DUA. There was also a significant lateral separation between the nearest downgradient freshwater aquatic life receptor location and the closest part of the groundwater plume. Remediation to Tier 1 was deemed unfeasible.

The area where the sulphur had been stored was on the higher elevation south and west parts of the site. Groundwater flow followed local topography and was radially outward to the east, northeast and north. Three 2-D numerical groundwater models were set up along three groundwater flowlines (approximately east, northeast and north), each passing through a part of the former source area.

The results of the numerical groundwater modelling for the status quo situation indicated that the sulphate concentration in the potential underlying DUA was predicted to exceed the drinking water guideline for sulphate in the future. Hotspots of sulphate contamination were iteratively removed from the model until the future drinking water guideline exceedance was no longer predicted to occur at any time. The hotspot areas removed from the model were used to develop a Remedial Action Plan by removing the equivalent volumes in the real world. The remediation plan developed to prevent future sulphate exceedance in the potential underlying DUA was sufficient to also prevent any future exceedance of the freshwater aquatic life guideline for sulphate at the closest downgradient location with the potential for groundwater discharge to a surface water body.

Conventional approaches including Tier 1 and Tier 2 guidelines were used to add areas to the remedial plan as needed to manage relatively small areas of other contaminants.

At the time of writing, the 3-year remedial program was approximately 50% complete.

1.2 Former Gas Plant Impacted by Sulfolane

MEMS developed a Residual Mass Based Remedial Plan based on numerical groundwater modelling for a former gas plant impacted with sulfolane in soil and groundwater.

The risk-based closure strategy was developed at the end of life of the facility but before the decommissioning of the surface facilities. The primary issue at the site requiring risk management was sulfolane in soil and groundwater beneath various parts of the former gas plant.

The CSM for the site identified source areas with sulfolane in shallow soil and two main plumes of sulfolane in groundwater extending downgradient from the source areas and comingling. A significant vertical separation was demonstrated between the base of sulfolane impact and the shallowest potential DUA. The groundwater plume extended off-site to the east beneath agricultural land. There was significant lateral separation between the nearest potential downgradient groundwater discharge point and freshwater aquatic life receptor location and the closest part of the groundwater plume.

Two 2-D numerical groundwater models were set up along two groundwater flowlines, each passing through one of the former source areas.

The results of the numerical groundwater modelling for the status quo situation indicated that remedial action was required to prevent future off-site migration of sulfolane in shallow groundwater at concentrations that would exceed the Tier 2 groundwater guideline protective of livestock watering if a dugout were constructed off-site in the future. No dugout is currently present on the adjacent property.

The risk-based actions supported by the numerical modelling included construction of a groundwater capture trench and treatment system along the downgradient property edge together with excavation and removal of soil impacted with sulfolane in source areas. The numerical modelling was used to confirm that implementing these actions driven by the protection of livestock exposure pathway would be sufficient to ensure protection of receptors *via* all other exposure pathways including the protection of DUA and freshwater aquatic life pathways, and also from other COPCs present at the site.

At the time of writing the groundwater interception trench and water treatment system had been constructed and were about to be commissioned, and the source remediation was approximately 50% complete.

1.3 Former Saltwater Storage Area

Matrix Solutions Inc. successfully achieved site closure at a former saltwater storage area using a Residual Mass Based Remedial Plan based on numerical groundwater modelling (Matrix, 2018).

A former saltwater storage area was surrounded by various receptors including class III and IV wetlands and overlying a domestic use aquifer (DUA). Groundwater chloride concentrations over 10,000 mg/L have been measured at the site.

A 3-D conceptual site model was developed for the site and used as a base to construct a regional scale 3-D numerical model encompassing the site and the main receptors (*i.e.*, the root zone, wetlands and DUA). The numerical model was calibrated to site specific data, including site observations of water levels, to successfully reproduce groundwater flow. The model was then used to simulate chloride transport. Several remedial scenarios (including excavation, barriers, site re-grading and pumping/ trench) were explored in the model to predict future chloride concentrations at receptor locations as a function of time and to assess the uncertainty of the predictions. This process was used to select the optimal remedial strategy which was shown to be an excavation within the rooting zone.

1.4 Chloride Impacted Wellsite

Matrix Solutions Inc. successfully achieved site closure at a chloride impacted wellsite using a risk-based closure strategy based on numerical groundwater modelling (Matrix, 2016).

A wellsite located in Alberta had salinity impacts distributed for approximately 16 m around the well head with chloride concentrations between 2,000 and 4,000 mg/L. The total mass of chloride was estimated to be relatively small, but the resources that would have been required to excavate the salinity impact would have been disproportionately large and appeared to be inappropriate when compared to the magnitude of the impact. Attempts to find a more practical remedial solution using the subsoil salinity tool were unsuccessful.

The site had over 10 years of data collected as part of various previous environmental site assessments. Geology consisted of over 20 m of silty clay with occasional discontinuous coarse-grained sand and gravel lenses of various sizes. Two areas north of the wellsite had been previously excavated as part of the remediation strategy. The objective of the study was to assess whether the contaminant left on site would pose a threat to receptors and whether additional remedial efforts were required.

A conceptual site model was developed for the site and expanded regionally to incorporate applicable receptors including private water wells and the most likely surface discharge location for groundwater (the Battle River).

Numerical models were developed to predict chloride concentrations as a function of time at various receptor locations. Three different models were used, each specific to the interface targeted. The Versatile Soil Moisture Budget (VSBM) model was used to model chloride transport within the root zone. Hydrus 1-D was used to model chloride transport through the unsaturated zone to the water table. A combination of FEFLOW, MODFLOW and MIKESHE (all 3-D saturated zone groundwater models) was used to model the saturated zone transport of chloride to the surface discharge location at the Battle River. Several case scenarios were run in the final model to predict chloride concentrations as a function of time at receptor locations and assess the uncertainty of the predictions.

Model results indicated that predicted chloride concentrations at receptor locations never exceeded regulatory threshold values and no further remediation was required to protect the receptors. The data were deemed sufficient and the uncertainty analysis was deemed to be adequate. Regulatory closure was obtained for the site from the Alberta Energy Regulator based on the Residual Mass Based Remedial Plan based on numerical groundwater modelling as described above. No post-closure groundwater monitoring was required at this site based on the groundwater monitoring already completed and the risk-based closure analysis provided.

2.0 EXAMPLES FROM OUTSIDE ALBERTA

Many possible examples exist, of which one is provided below.

2.1 Rotterdam Harbour - Netherlands

The Rotterdam Megasite is located in the Netherlands and is the world's largest harbour. Activities including transshipment and processing of bulk goods such as oil, chemicals, coals and ores have resulted in groundwater contamination over much of the harbour. Activities in the harbour have been on-going since the 1800s and it is unrealistic and unrequired to expect a complete remediation of the area. However, the site was required to comply with the requirements of the European Union (E.U.) Water Framework Directive and Groundwater Directive which committed members to achieve good qualitative and quantitative status of all water bodies by 2015. Deltares (2019) described a Remedial Mass Approach that was used for this site based on numerical groundwater modeling. An agreement was reached between the Authorities (E.U.) and local stakeholders for the remediation and management of the contaminated lands and groundwater.

The steps included developing an integrated management strategy (IMS) encompassing aspects of risk assessment and risk management. The groundwater numerical modelling informed the risk assessment and risk management portions of the IMS. A risk management zone (RMS) was selected and delineated by planes of compliance, defined as the boundaries of receptors to be protected. The plane of compliances included the interface between groundwater and surface water, an aquifer located directly below the harbour and pristine groundwater systems located outside the harbour area.

Groundwater numerical modelling was completed using MODFLOW and transport modelling tools such as MT3D, RT3D and MODPATH (a particle tracking tool). A proprietary piece of software was used to process the output results from MODFLOW and MODPATH and to calculate biodegradation with time at the planes of compliance. The modelling outputs included the calculated contaminant concentrations and mass fluxes at the three planes of compliance, presented for different moments in time (past, present and future). Uncertainty in the modelling results was assessed using a Monte-Carlo analysis simulating many different modelling outcomes and assessing the relative sensitivity of model outcomes to various parameters.

Contaminant concentrations as predicted by the numerical model were compared with pre-defined risk-based screening levels. Impacts at the planes of compliance were estimated as the surface area with concentrations above the screening levels, at a defined point in time. Maps were created illustrating the spatial distribution of contaminants and the probability of exceeding screening values at given points in time for the aquifers located below the harbour and outside the harbour. Modelling results indicated the aquifer below the harbour is already impacted and concentrations will increase with time before stabilizing. Results also indicated that groundwater systems outside the harbour are not yet impacted but will be in the future.

The model helped with characterizing contaminant distribution and migration, indicated that natural attenuation would be insufficient to protect groundwater systems outside the harbour and demonstrated that active measures were required to reverse the current trend and protect the aquifers outside of the harbours.

The groundwater numerical model was further used to assess the effectiveness of various risk management (remediation) scenarios that would be implemented to protect the unimpacted groundwater systems. The risk reduction effect and the costs of the basic management scenarios were assessed during the exercise. An approach based on combined remediation strategies was selected as the optimum path to meet both the Regulatory and stakeholder requirements.

This example is useful and relevant to the current study because it illustrates how the principles proposed in this document have been employed in other parts of the world and accepted as pragmatic solutions to complex contaminant problems by other regulatory jurisdictions.

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APPENDIX B: REGULATORY GUIDANCE ON NUMERICAL MODELLING

Appendix B

Regulatory Guidance on Numerical Modelling

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This appendix summarizes a part of the large body of documentation on groundwater modelling available from regulatory jurisdictions in Canada, the United States, and other countries. Table B-1 presents a summary of selected guidance documents available for these regions.

Many of these reports contain detailed guidance on constructing a numerical groundwater model. This information is of some relevance to the current work. Much of the information is similar between the various documents. Some of the documents are written to provide guidance for regulatory reviewers of groundwater models.

1.0 CANADA

1.1 Alberta

The only document on groundwater modelling specific to the Province of Alberta is a report by the Cumulative Environmental Management Association (CEMA, 2012) and was written specifically for projects in the Alberta Oil Sands. This document provides a detailed description of how to construct a numerical groundwater model to support Environmental Impact Assessments of Oil Sand projects. The report discusses a range of groundwater model codes including MODFLOW, FEFLOW and HSPF and also considers models that couple groundwater and surface water (such as MIKE SHE or GS-FLOW).

Table B-1 Regulatory Guidance Documents on Modelling			
Publisher	Date	Title	Reference
Canada			
British-Columbia Ministry of Environment – Water Protection & Sustainability Branch	2012	Guidelines for Groundwater Modelling to Assess Impacts of Proposed Natural Resource Development Activities	BCMoe (2012)
CEMA (Cumulative Environmental Management Association)	2012	Alberta Oil Sands Groundwater Modelling Guidelines (Unpublished)	CEMA (2012)
United States			
U.S. EPA (United States Environmental Protection Agency)	1992	Fundamentals of Ground-Water Modeling	Bear <i>et al.</i> (1992)
U.S.G.S. (U.S. Geological Survey)	2004	Guidelines for Evaluation Groundwater Flow Models	Reilly and Harbaugh (2004)
U.S.G.S. (U.S. Geological Survey)	1998	Methods and Guidelines for Effective Model Calibration	Hill (1998)
ASTM (American Society for Testing and Materials)	2000	Standard Guide for Subsurface Flow and Transport Modelling. ASTM D5880-95(2000)	ASTM (2000)
ASTM (American Society for Testing and Materials)	2013	Standard guide for Documenting a Groundwater Flow Model Application. ASTM D5718-13	ASTM (2013)
ASTM (American Society for Testing and Materials)	2014	Standard guide for Conceptualization and Characterization of Groundwater Systems. ASTM D5979-96(2014)	ASTM (2014a)
ASTM (American Society for Testing and Materials)	2014	Standard Guide for Developing Conceptual Site Models for Contaminated Sites. ASTM E1689–95(2014)	ASTM (2014b)
ASTM (American Society for Testing and Materials)	2014	Standard Guide for Defining Initial Conditions in Groundwater Flow Modelling. ASTM D5610–94(2014)	ASTM (2014c)
ASTM (American Society for Testing and Materials)	2014	Standard Guide for Comparing Groundwater Flow Model Simulations to Site-specific Information. ASTM D5490–93(2014)e1	ASTM (2014d)

Table B-1 Regulatory Guidance Documents on Modelling			
Publisher	Date	Title	Reference
ASTM (American Society for Testing and Materials)	2016	Standard Guide for Defining Boundary Conditions in Ground-Water Flow Modeling. ASTM D5609-16	ASTM (2016a)
ASTM (American Society for Testing and Materials)	2016	Standard Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application. ASTM D5611-94(2016)	ASTM (2016b)
ASTM (American Society for Testing and Materials)	2017	Standard Guide for Selecting a Groundwater Modelling Code. ASTM D6170-17	ASTM (2017a)
ASTM (American Society for Testing and Materials)	2017	Standard Guide for Application of a Groundwater Flow Model to a Site-specific Problem. ASTM D5447-17	ASTM (2017b)
ASTM (American Society for Testing and Materials)	2018	Standard Guide for Calibrating a Ground-Water Flow Model Application. ASTM D5981/D5981-18	ASTM (2018)
Alaska Department Of Environmental Conservation Division of Spill Prevention and Response Contaminated Sites Program	2017	Fate and Transport Modeling Guidance	Alaska DEC (2017)
State of Ohio – Environmental Protection Agency	2007	Ground Water Flow and Fate and Transport Modeling	Ohio EPA (2007)
Georgia Department Natural Resources Environmental Protection Division Land Protection Branch	2016	Guidance: Groundwater Contaminant Fate and Transport Modeling	Georgia DNR (2016)
Michigan Department of Environmental Quality Remediation and Redevelopment Division Resource Materials	2014	Groundwater Modeling.	Michigan DEQ (2014)
Other Regions			
Australian Government National Water Commission	2012	Australian Groundwater Modelling Guidelines	Australian GNWC (2012)

Table B-1 Regulatory Guidance Documents on Modelling			
Publisher	Date	Title	Reference
BRGM (Bureau de Recherches Géologiques et Minières)	2016	Modélisation maillée des écoulements souterrains Principes, démarche et recommandations	French BRGM (2016)
National Groundwater and Contaminated Land Centre	2001	Guide to Good Practice for the development of Conceptual Models and the Selection and Application of Mathematical Models of Contaminant Transport Processes in the Subsurface	U.K. NGCLC (2001)

1.2 British Columbia

The British Columbia Ministry of Environment (BC MoE, 2012) has published a guidance document intended to support modelling projects associated with resource industries in British Columbia. The guidelines indicate how groundwater models can be used to evaluate the potential impacts of a project and identify mitigative measures to the groundwater system and associated receptors. The guidelines also cover in detail the steps required to develop a groundwater model, including developing a conceptual site model, selecting a mathematical model, constructing and calibrating the model, running scenarios to obtain predictions and assessing model sensitivity and uncertainty. The last two sections of the BC MoE guidelines are of particular relevance to the current project as they address model documentation and review. There is much useful material here which has informed the content of this report.

2.0 UNITED STATES

Numerous United States Federal and State guidance documents exist and range in content from highly technical to more general and practical coverage.

The U.S. Environment Protection Agency (U.S. EPA) and U.S. Geological Survey (U.S.G.S.) published some of the earliest guidance on how to construct and apply numerical groundwater models. The three documents listed in Table 1 form a reference point that is drawn on by many of the other documents in this Section. Of particular relevance to the current work is the 2004 U.S.G.S. report that is written as a resource for reviewers of groundwater models, and material from this report informed the current work

The American Society for Testing and Materials (ASTM) documents are very technical and are considered a standard reference for many aspects of groundwater modelling. These documents were published in the United States but are used by a world-wide audience.

The State-specific groundwater modeling guidelines typically derive their content from the U.S. EPA and U.S.G.S general guidance documents and from the ASTM Standards, and contain little new material. Most of the documents include the same core sections including defining clear objective for the model, developing a conceptual site model, choosing an appropriate modelling tool, developing and calibrating the model, running predictive scenarios, assessing model sensitivity and uncertainty and drafting a modelling report.

3.0 OTHER JURISDICTIONS

Guidance documents on numerical modeling were available for the United Kingdom, France and Australia. Groundwater modelling guidance documents may well exist in other regulatory jurisdictions but were not consulted in the review for the current work.

The French guidance document focuses on groundwater flow modelling, from simple to very complex, and from very small scale to very large scale. The document focuses on the best approach to develop models for data intensive areas and very complex models, to avoid pitfalls. Models developed in France are often used for the management of water resources and thus have a degree of complexity that is generally higher than the smaller scale model used for impact assessment or to test remediation scenarios. The document presents a rigorous approach to groundwater modelling to achieve reliable models for water management.

The U.K. guidance document focuses on the use of groundwater models in the context of risk assessment and the remediation of contaminated groundwater. Emphasis is placed on model codes and equations simulating the transport of aqueous-phase contaminants in the unsaturated and saturated zones to determine impact on groundwater and surface water receptors. The purpose of the document is to provide a general good practice approach to contaminant fate and transport modelling from setting objectives to the interpretation of results and model validation.

The Australian guidance document addresses both groundwater flow and contaminant transport modelling to promote consistency in groundwater modeling in Australia.

Guidance documents from the United Kingdom, France and Australia cover similar topics as guidance documents from Canada and the U.S. demonstrating consistency on what is considered best practice for developing groundwater models, regardless of the country or final use (water management, contaminant transport, impact assessment) of the model.

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