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Best Management Practices for Using Numerical Modelling Approaches in Contaminated Sites Management

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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 managing contaminated sites to 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.

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 conservatism associated with applying Tier 1 and Tier 2 guidelines can become a major impediment to developing an economically viable contaminant management strategy at large and complex contaminated sites where groundwater pathways are the primary risk drivers.

Numerical groundwater models can be used to provide contaminant management strategies 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.

For the purposes of this document the term “Numerical Model Approach” refers to a contaminant management strategy based on the results of numerical groundwater model.

1.1 Objective

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

1.2 Acknowledgements

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2.0 REGULATORY CONTEXT AND APPLICATION

2.1 Regulatory Applicability

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

2.2 Source Control

Source control is one of the fundamental principles of contaminant management in the Alberta Contaminated Sites Framework (ESRD, 2014). Removal or control of sources of contamination is always required before other risk-based tools are applied, and this principle applies just the same when numerical model approaches are used. Nothing in this document supersedes the regulatory requirement for source control.

2.3 Conservatism

The Tier 1 and Tier 2 guideline framework makes use of conservative assumptions to offset the uncertainty involved in using a relatively small number of measurements to make predictions on how contaminants will move in the subsurface. The same approach is required for numerical model approaches, where conservative assumptions are still needed to offset the level of uncertainty associated with the dataset being used. In general, the smaller the dataset available for a particular model input parameter, the greater the need for conservatism in selecting an appropriate parameter value. As the size of the dataset increases, there is a greater confidence that the available data adequately characterize the heterogeneity of the subsurface and the degree of conservatism can be adjusted accordingly.

2.4 Applications of Numerical Model Approaches

The purpose of building a numerical model for contaminated site management is to predict future contaminant concentrations at exposure points based on the current distribution of contaminant in the subsurface. There are three main applications of this process within the Alberta Contaminated Sites Framework. These are to support the development of:

- remedial action plans;
- risk management plans; and
- site closure plans.

Much of the information in this report applies equally to all three approaches, but information specific to these three applications is provided in Section 6.

2.5 Regulatory Acceptance and Consultation

For contaminated sites within the jurisdiction of the Alberta Energy Regulator, guidance on when regulatory acceptance and/or consultation may be available is provided in Manual 021 (AER, 2021). Nothing in this document supersedes the guidance in Manual 021 which applies equally to numerical model-based approaches.

3.0 PROBLEM STATEMENT

This project proposes best management practices for managing contaminated sites based on numerical modelling approaches. Key aspects of these approaches are expanded in the following sections.

3.1 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 chemical of potential concern being present at 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.

3.2 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, or risk management measures are required.

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.

3.3 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.

3.4 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 large size and complexity of contaminant plume.

3.4.1 Groundwater Pathways Driving Remediation

Tier 1 and 2 guidelines are typically calculated for a range of exposure pathways (see Section 3.1). 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 or risk management plans.

3.4.2 Contaminant Type

Appendix A provides examples where Numerical Model Approaches have been used successfully at real-world sites to support remedial action plans, risk management plans, and/or site closure plans. The examples in Appendix A 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.

3.4.3 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. 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.

3.5 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 Numerical Model Approaches will help standardize approaches and assumptions across the industry and may support the development of high-quality reports.

4.0 BACKGROUND INFORMATION

4.1 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.

4.2 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.

4.3 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 1-, 2- or 3-dimensional model volume.

4.4 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 at are calculated for each Timestep in each Model Cell.

4.5 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: 1-D, 2-D, or 3-D. Most model codes can accommodate 3-D 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 3-D 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 4.3 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).

4.6 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.
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.

Table 1 Modelling Codes Commonly Used in Canada

Model Code	Type	Overview
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 models 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 MODEL CONSTRUCTION AND VALIDATION – BEST MANAGEMENT PRACTICES

The Best Management Practices in this section are intended to provide guidance to proponents constructing and validating numerical models in contaminated site management, 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).

As indicated in Section 4.2, 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. 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. Information provided in this section is intended to provide Best Management Practices when Numerical Modelling Approaches are used to support contaminant management strategies.

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

- address preliminary questions;
- develop/refine Conceptual Site Model;
- set up numerical model;
- conduct groundwater flow calibration and verification;
- conduct transport model selection, predictions and verification; and
- undertake uncertainty assessment/ sensitivity analysis.

Best Management Practices information for each of these steps is provided in the following Sections. Where appropriate, specific points to be addressed by the modeller or checked by the reviewer are highlighted by bullets.

5.1 Preliminary Questions

5.1.1 Identify Model Objective and Problem to be Solved

The first step in developing a Numerical Model Approach is to check that the objective is clearly defined. 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 objective will be to use a Numerical Model Approach to determine the remedial or risk management measures that will be required to protect 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. The selection of chemical(s) to be modelled and receptor locations to be assessed must be clearly identified and justified.

5.1.2 Determine Appropriateness of Numerical Model Approach

The appropriateness of using a Numerical Model Approach at the site should be clearly justified. Section 3.4 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 or if groundwater-mediated pathways are driving risk after other pathways are managed.
- Contaminant(s) driving remediation are soluble and non-degrading.
    - Numerical models can be used for degrading chemicals, but 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.

5.1.3 Ensure Adequate Data are Available

A Numerical Model Approach is a type of site-specific risk assessment (SSRA) as defined in the Tier 2 guidelines document (AEP, 2019b). An SSRA is a more comprehensive assessment than Tier 1 or Tier 2 guideline modification approaches, and therefore it is expected that more comprehensive data will be collected to support this approach. Professional judgement is required to assess the adequacy of the data set used to build a numerical model. Relevant information should be provided, including an evaluation of potential gaps and any assumptions made to fill gaps should be clearly indicated.

Numerical Model Approaches meeting Best Management Practices will tabulate all model input parameter values to indicate clearly:

- The range and number of measured values.
- The initial parameter value used in the numerical model.

- The final model parameter value selected after model calibration.

Where different model parameters are used for different units or zones in the numerical model, the above information is required for each unit or zone.

5.2 Conceptual Site Model

A critical step in constructing an acceptable numerical model is the development of a conceptual site model (CSM). The CSM required 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.*

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.

Numerical Model Approaches meeting Best Management Practices will include, at a minimum, the following CSM 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 the main geological and hydrogeological units expected to control contaminant transport, 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.

The conceptual site model (CSM) should include enough information to support the building of a credible numerical model to support remediation planning, risk management planning and/or site closure. Additional material that does not relate to these needs is not helpful and detracts 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 given site. Increased delineation is always possible, but the appropriate assessment standard is whether delineation is sufficient to provide confidence that contaminated site management decisions based on a Numerical Model Approach will adequately protect receptors from current tor future adverse effects.

Required CSM components are discussed in the following sections.

5.2.1 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 5.2.3) are appropriate. Summary information on topography and nearby surface water bodies will help understand whether the appropriate exposure pathways have been considered (Section 5.2.4).

5.2.2 Geological and Hydrogeological Units

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the bullet points in this section:

- 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.

5.2.3 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 need 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.

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the following bullet points:

- 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?

5.2.4 Exposure Pathways and Associated Receptors

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the following bullet points:

- Are the applicable exposure pathways and associated receptors identified for the COPCs noted above?

- Is the limiting pathway for the chemical(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)?

5.3 Model Set-Up

Once the CSM is satisfactory, the next step is to set up the model. Typically, the following steps will be needed.

5.3.1 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.

5.3.2 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 as well as the top and bottom 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. Overall, the boundary conditions should make physical sense in relation to the real-world situation and should allow for a reasonably accurate calibration of the flow model to real world data.

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.

5.3.3 Numerical Model Validity Criteria

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

5.3.3.1 Model Domain and Cell Size

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

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the bullet points in this section:

- 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 will normally need 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.

5.3.3.2 Boundary Conditions

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the bullet points in this section:

- 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 flow model calibration will be achievable (Section 5.4).

5.3.3.3 Hydraulic Properties

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the questions in the bullet points in this section:

- Is a rationale provided for the initial hydraulic properties used in the model and are these clearly tabulated for initial values and calibrated values 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, and both initial and calibrated values should be clearly identified and tabulated and should be within physically reasonable ranges based on the stratigraphy defined and the climatic conditions for the site location.

5.4 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 for the hydraulic properties of each layer and the 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) sufficiently detailed 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.

A typical workflow for groundwater flow modelling involves imposing initial values of hydraulic properties on the model defined by the model domain and boundary conditions 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 until an acceptable match is achieved, and the flow model is considered to be calibrated.

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the following questions:

- 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 contaminant management strategies based on a Numerical Model Approach are likely to achieve their 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.

5.5 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, fully quantitative validation of a transport model will not be possible. However, constraints on the time window when a release could have occurred (e.g., not before the facility became operational, or not after the time when the use of a particular chemical was discontinued) can still be helpful in determining whether the general size and location of the currently observed contaminant plume are broadly consistent with the model.

Often the best available solution will be to superimpose the known, current contaminant distribution on top of a calibrated flow model and run the model 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 Alberta Tier 1 and Tier 2 guidelines have adopted 500 years as the appropriate length of time to model future groundwater transport of contaminants in groundwater for the purposes of setting remediation guidelines. The same timeframe is appropriate for Numerical Model Approaches.

Once the transport model is built, the recommended approach to transport model validation is to incrementally build levels of confidence in the model results by incorporating as many as possible of the following weight of evidence transport model validation points:

- Goodness of fit of modelled against measured piezometric heads (flow model calibration).
- Semi-quantitative transport model validation based on the assumed time of release and the current plume size.
    - It will generally not be possible to reproduce the current plume distribution from information about the original source, but it may be possible to demonstrate that the magnitude of the current plume is plausible, or at least not inconsistent with available information or constraints on source location, intensity and timing.

- Long-term trends in monitoring well data can be used to infer the rate of plume movement and help with validation against modelled plume movement.
- The size and quality of the dataset for hydraulic conductivity, bulk density/porosity and fraction of organic carbon can provide confidence that model inputs used are indeed representative of the bulk properties of the unit in question.
- Sensitivity analysis can be used to help understand the consequence on model conclusions of uncertainty in key model input parameters.
- The use of conservatism in model assumptions can help to account for uncertainty.

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the following questions:

- 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?
- Is there sufficient weight of evidence from information provided relative to the transport model validation points indicated above to have adequate confidence in the results of the transport model?

5.6 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.

5.7 Model Reporting and Output

Model reporting should address all of the Best Management Practices points highlighted in the document. It should summarize the conceptual site model and provide a succinct summary of salient elements of how the model was build and the rationale for doing so. Model parameters should be tabulated, with clarity as to the initial values used and the final values adopted after flow model calibration. 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 how the transport model was conducted and the ways in which the factors indicated in Section 5.5 were used to incrementally build levels of confidence in the model results. 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. A report section addressing model assumptions is required.

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the following questions:

- 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.

6.0 APPLICATIONS IN CONTAMINATED SITE MANAGEMENT

As indicated in Section 2.4, the numerical modelling techniques discussed in this document have potential applications in developing remedial action plans, risk management plans, and site closure plans. Information provided in preceding sections of this report is equally applicable to all three of these applications. The following sub-sections provide guidance on using numerical model results in these three applications.

6.1 Remedial Action Plans

The groundwater flow and transport model discussed 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.

Numerical Model Approaches meeting Best Management Practices will provide acceptable answers to the following questions:

- 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?

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 significantly 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 original effort required to build the model, and there is a clear advantage in knowing if any 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.

6.2 Risk Management Plans

The groundwater flow and transport model created in Section 5 can also be used to support a risk management plan for the site. In this case, exposure point locations with current or future predicted concentrations that exceed exposure thresholds for particular receptors indicate situations that require risk management measures to be implemented. The magnitude and timing of predicted future exceedances can be used to inform decisions about the risk management measures that will be required and the length of time that the risk management measures may need to be maintained.

In some cases, it may be appropriate to use a Numerical Model Approach to support a hybrid process where accessible areas of contamination are remediated, while risk management measures are implemented to protect receptors from the effects of contaminants in areas that may not be currently accessible due to the presence of active infrastructure or for other reasons.

6.3 Site Closure

In cases where the groundwater flow and transport model created in Section 5 does not predict any current or future contaminant concentrations that exceed exposure limits at locations where receptors could be exposed, it may be possible to move towards site closure based on numerical model results.

6.4 Other Considerations

Sites that proceed to a remedial action plan, risk management plan or site closure based on 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 this document helps develop a 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 exposure pathways as well.

Numerical Model Approaches meeting Best Management Practices will provide an acceptable answer to the following question:

- 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?

6.5 Summary and Conclusion

This document provides guidance on Best Management Practices for using Numerical Model approaches to support remedial action plans, risk management plans and site closure. If the guidance in this document is followed, and acceptable answers are provided to the Best Management Practice bullet points provided, then there is an acceptable level of confidence that the remedial action plan, risk management plan or site closure proposal based on the Numerical Model Approach will achieve receptor protection goals consistent with EPEA requirements.

7.0 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 Agreements for PTAC Project references 18-RRRC-03, 19-RRRC-07 and 20-RRRC-12. This report does not necessarily represent the views or opinions of PTAC or the PTAC members.

Transport modelling involves a number of uncertainties and limitations. As a consequence, the use of the process presented herein to develop site management strategies may either be overly protective or may not necessarily provide complete protection to human receptors or prevent damage of property in all circumstances. The process presented herein was determined in accordance with generally accepted protocols. Given the assumptions indicated, the process presented herein is expected to provide a conservative estimate of the risks involved. The services performed in the preparation of this report were conducted in a manner consistent with the level of skill and care ordinarily exercised by professional engineers and scientists practising under similar conditions.

While preparing this report, Millennium may use or incorporate Millennium's proprietary algorithms, methods, compilations, processes, designs, formulas, and/or techniques, and may also employ advanced technologies for simulation, information modeling, generative design, and the development of project documentation (the "Technical Tools"). The Technical Tools may be further used to create data sets and result in simulations or models (collectively, the "Datasets") that may be included in this report. Both the Technical Tools and the Datasets are by-products of Millennium's internal processes and shall belong solely to Millennium. No unauthorized use of the Technical Tools or Datasets is permitted.

The results and interpretations included in this report do not represent any specific site. Millennium accepts no responsibility for foreseeable or unforeseeable damages, or direct or indirect damages, if any, suffered by any third party as a result of decisions made or actions taken based on the use of this report, including but not limited to damages relating to delay of project commencement or completion, reduction of property value, and/or fear of, or actual, exposure to or release of toxic or hazardous substances.

Yours truly,

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8.0 REFERENCES

AEP (Alberta Environment and Parks), 2019a. Alberta Tier 1 *Soil and Groundwater Remediation Guidelines*. Land and Forestry Policy Branch, Policy Division. 195 pp.

AEP (Alberta Environment and Parks), 2019b. Alberta Tier 2 *Soil and Groundwater Remediation Guidelines*. Land and Forestry Policy Branch, Policy Division. 151 pp.

AER (Alberta Energy Regulator), 2021. Manual 021: Contamination Management. October 2021.

Australian Government National Water Commission. 2012. Australian Groundwater Modelling Guidelines. Sinclair Knight Merz and National Center for Groundwater Research and Training. Waterlines Report Series No.82. June 2012.

Bear J., M.S. Beljin and R.R. Ross. 1992. Fundamentals of Groundwater-Modeling. US EPA Groundwater Issue. EPA/540/S-92/005. April 1992.

British Columbia Ministry of Environment (BC MoE). 2012. Guidelines for Groundwater Modelling to Assess Impacts of Proposed Natural Resource Development Activities. Water Protection & Sustainability Branch. April 2012.

CEMA (Cumulative Environmental Management Association), 2012. Alberta Oil Sands Groundwater Modelling Guidelines. *Unpublished* – November 2012.

ESRD (Alberta Environment and Sustainable Resource Development), 2014. Contaminated Sites Policy Framework. Land and Forestry Policy Branch, Policy Division, 25pp.

Government of Alberta, 2017. *Environmental Protection and Enhancement Act*. Revised Statutes of Alberta 2000, Chapter E-12. Current as of December 15, 2017. Alberta Queen's Printer.

Konikow, L.F. 2011. The Secret to Successful Solute-Transport Modeling. Ground-Water. Vol. 49, No.2. March-April 2011. Pp 144-159.

USGS (United States Geological Survey), 2004. Guidelines for Evaluating Ground-Water Flow Models. Scientific Investigations Report 2004-5038. 30 p.

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

Appendix A – Examples of Site Closure Based on Numerical Model Approaches

Table of Contents

This Appendix provides examples where Numerical Model Approaches have achieved regulatory acceptance to support remedial action plans, risk management plans, and site closure plans 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 has achieved regulatory acceptance of a combined remedial action plan and risk management plan based on a Numerical Model Approach 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 a combination of risk management measures and remedial action were required to prevent future off-site migration of sulfolane in shallow groundwater and to ensure all potential receptors were adequately protected.

The risk management measures supported by the numerical modelling included construction of a groundwater capture trench and treatment system along the downgradient property edge together with restrictions on constructing a dugout within the affected area. Remedial actions supported by the numerical modelling included a series of excavations of soil impacted with sulfolane in source areas. The groundwater capture trench and treatment system will also contribute to remedial efforts by reducing the mass of sulfolane in groundwater.

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.

1.3 Former Saltwater Storage Area

Matrix Solutions Inc. successfully achieved site closure at a former saltwater storage area by implementing a Remedial Action 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 Numerical Model Approach (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 transhipment 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 MODLOW 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 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.

3.0 REFERENCES

AENV (Alberta Environment), 2011. Guidelines for Landfill Disposal of Sulphur Waste and Remediation of Sulphur Containing Soils. September 2011. 39 pp.

Deltares. 2019. Integrated Management Strategy, Examples – Rotterdam. Accessed on January 14, 2019 at: https://publicwiki.deltares.nl/display/IMSW/Rotterdam+-+Starting+IMS

Matrix Solutions Inc. 2016. Routine Site Closure Supported by Numerical Modelling. Presented at the Exova Seminar on January 15, 2016.

Matrix Solutions Inc. 2018. Developing the Insights Required for Informed-Decision-Making at Salt-Impacted Sites. Presented at RemTech 2018, Banff, AB on October 12, 2018.

APPENDIX B: REGULATORY GUIDANCE ON NUMERICAL MODELLING

Appendix B – Regulatory Guidance on Numerical Modelling

Table of Contents

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 *et al*. (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)

Table B-1 Regulatory Guidance Documents on Modelling

Publisher	Date	Title	Reference
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)
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)

Table B-1 Regulatory Guidance Documents on Modelling

Publisher	Date	Title	Reference
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)
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.

4.0 REFERENCES

Alaska Department of Environmental Conservation. 2017. Fate and Transport Modeling Guidance. Division of Spill Prevention and Response Contaminated Sites Program. January 2017.

ASTM (American Society for Testing and Materials), 2000. Standard Guide for Subsurface Flow and Transport Modelling. ASTM D5880-95(2000).

ASTM (American Society for Testing and Materials), 2013. Standard guide for Documenting a Groundwater Flow Model Application. ASTM D5718-13.

ASTM (American Society for Testing and Materials), 2014a. Standard guide for Conceptualization and Characterization of Groundwater Systems. ASTM D5979-96(2014).

ASTM (American Society for Testing and Materials), 2014b. Standard Guide for Developing Conceptual Site Models for Contaminated Sites. ASTM E1689–95(2014).

ASTM (American Society for Testing and Materials), 2014c. Standard Guide for Defining Initial Conditions in Groundwater Flow Modelling. ASTM D5610–94(2014).

ASTM (American Society for Testing and Materials), 2014d. Standard Guide for Comparing Groundwater Flow Model Simulations to Site-specific Information. ASTM D5490–93(2014)e1.

ASTM (American Society for Testing and Materials), 2016a. Standard Guide for Defining Boundary Conditions in Ground-Water Flow Modeling. ASTM D5609-16.

ASTM (American Society for Testing and Materials), 2016b. Standard Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application. ASTM D5611-94(2016).

ASTM (American Society for Testing and Materials), 2017a. Standard Guide for Selecting a Groundwater Modelling Code. ASTM D6170-17.

ASTM (American Society for Testing and Materials), 2017b. Standard Guide for Application of a Groundwater Flow Model to a Site-specific Problem. ASTM D5447-17.

ASTM (American Society for Testing and Materials), 2018. Standard Guide for Calibrating a Ground-Water Flow Model Application. ASTM D5981/D5981-18.

Australian Government National Water Commission. 2012. Australian Groundwater Modelling Guidelines. Sinclair Knight Merz and National Center for Groundwater Research and Training. Waterlines Report Series No.82. June 2012.

Bear J., M.S. Beljin and R.R. Ross. 1992. Fundamentals of Groundwater-Modeling. US EPA Groundwater Issue. EPA/540/S-92/005. April 1992.

British Columbia Ministry of Environment (BC MoE). 2012. Guidelines for Groundwater Modelling to Assess Impacts of Proposed Natural Resource Development Activities. Water Protection & Sustainability Branch. April 2012.

Bureau de Recherches Géologiques et Minières. 2016. Modélisation Maillée des Écoulements Souterrains Principes, Démarches et Recommandations. Rapport Final – Version 2. BRGM/RP-62549-FR. Octobre 2016.

Cumulative Environmental Management Association (CEMA). 2012. Alberta Oil Sands Groundwater Modelling Guidelines. *Unpublished* – November 2012.

Georgia Department of Natural Resources. 2016. Guidance: Groundwater Contaminant Fate and Transport Modeling. Environmental Protection Division. Land Protection Branch. October 2016.

Michigan Department of Environmental Quality. 2014. Groundwater Modeling Remediation and Redevelopment Division Resource Materials. February 2014.

Reilly T.E. and A.W. Harbaugh. Guidelines for Evaluating Ground-Water Flow Models. U.S. Geological Survey. U.S. Department of the Interior. Scientific Investigation Report 2004-5038.

State of Ohio Environmental Protection Agency. 2007. Ground Water Flow and Fate and Transport Modeling. Division of Drinking and Ground Waters. Technical Manual for Ground Water Investigations Chapter 14. November 2007.