A Guide for Actively Managing Watershed-Scale Numerical Models in Ontario

OakRidgesMoraine GROUNDWATER PROGRAM

$$\frac{\partial}{\partial x}\left(K_x(\theta)\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(\theta)\frac{\partial h}{\partial y}\right)+$$

$$\frac{\partial q_x}{\partial t}+\frac{\partial}{\partial x}\left(uq_x\right)+\frac{\partial}{\partial y}$$

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August, 2017

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This guide has been prepared by staff from the Oak Ridges Moraine Groundwater Program (ORMGP; formerly known as YPDT-CAMC Groundwater Management Program) based on experiences with data management and numerical modelling over the past 20 years. The ORMGP study team was augmented by Thorsten Arnold who contributed a knowledge management perspective for organising complex modelling workflows. The report was supported and financed with provincial funding allocated through the Credit-Toronto-Central Lake Ontario (CTC) and Lake Erie Source Water Protection programs.

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FOREWORD

The use of numerical computer models to represent the storage and transmission of water in the terrestrial phase of the hydrological cycle has been validated as a central and essential analytical approach in water management practice and policy development in Ontario. The capability of models to assess the effects of water takings, land-use changes, and climate trends on water distribution has been demonstrated through the successful completion of Water Budget and Stress Assessment Reports for much of southern Ontario to satisfy requirements of the Clean Water Act, 2006.

Numerical models are now unsurpassed for decision-making in water allocation, protection of water sources, and for risk-reduction policies for extreme conditions (e.g., flood and drought). Acting on this, recognition, preparation, and use of numerical models is now routinely required for various water resources management initiatives across the province.

The workflows inherent in numerical modelling, specifically the need for the assembly, review, analyses, and syntheses of large collections of data, results in a tremendous synthesis of water resources information. This synthesis is an ongoing activity that builds on advances in knowledge in both field measurements and improved model algorithms.

Numerical modelling must be recognised as a continuing, iterative, and evolving process. Accordingly, model management plans must be aligned with this thinking. To capitalise on the investment in modelling work undertaken to date, and to ensure efficiency in the continued advance toward more effective water management for the long-term, it is incumbent upon agencies commissioning modelling studies to put in place practices to effectively manage the numerical models and attendant data sets to facilitate continued use and improvement of the models going forward.

It is intended that this guide will raise awareness of the need to reposition Ontario's water managers to integrate numerical modelling as a standard water management tool for developing policies, infilling data gaps, impact assessment, scenario analyses, communicating the behaviour of complex environmental systems to stakeholders, and decision making with regards to a wide range of water resources concerns. It is also intended to equip water managers with the 'know how' to effectively manage the numerical modelling pathway so that Ontario may capitalise on the full potential of numerical modelling.

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1 INTRODUCTION

1.1 PURPOSE

The document is intended to provide model-related guidance that will lead to the increased understanding, comfort, and ultimate utility of numerical models by public sector agencies in Ontario. As such, the document is written largely for public sector agency staff (at provincial, municipal, or conservation authority levels) who might be involved in the commissioning or management of numerical modelling studies. The managers of these studies may or may not have access to technical modelling knowledge and the guide therefore generally follows a progression from simpler to increased technicality suited to the needs of the reader. This document is intended to guide high-level managers in making sound, far-sighted water-related decisions while managing public funds responsibly. At the same time, it also outlines the technical details and workflows that modelling consultants will deliver during model development. As the focus of this guide is to provide model management guidance, it avoids presenting the detailed technical knowledge required by the modelling community. To explore such in-depth knowledge, readers are invited to review the literature cited throughout the guide as well as the publications included in the annotated bibliography (Appendix 2).

This guide provides an overview of the basic recommended steps for organisations to follow when commissioning numerical modelling studies, with the intention of introducing standardised environmental modelling terminology and clarifying the technical steps required for effective high-level model management as well as data and knowledge transfer. The guide will assist model managers with assessing data needs, with respect to: i) the data they must assemble prior to and in support of model development; ii) the interpretations of these data that may be required for modelling; and iii) the data, model files, and results they should expect once the completed models are delivered. Effective data management ensures that model development costs remain low and that modelling proceeds within scope and set schedules, and also assists in preserving the utility of the delivered model for future use.

It is anticipated that the guide will constitute a thorough reference aimed at those responsible for commissioning and managing numerical modelling studies. Through this guide, it is anticipated that a sound model management practice will lead to a reduction in water management–related costs by:

- providing the opportunity for public sector agency staff to become more familiar with modelling terminology and processes such that they have a clear appreciation for:
    - data requirements needed in support of a modelling study,
    - the expected costs both in terms of finances and time commitments, and
    - the expected results from a numerical model (i.e., model applicability, model limitations, etc.);
- providing examples of contract clauses that can direct consultants at the onset of modelling studies for public sector agencies; and
- describing a model management system that will:
    - improve the use of existing numerical models (or elements of them),

- improve data management in support of current and future numerical modelling,
- optimise the process of managing, maintaining, and repurposing previously commissioned numerical models, and
- improve the communication of knowledge that is generated through the numerical modelling process.

Although this guide is largely directed towards regional-scale water budget–type models similar to those built for Ontario's source water protection (SWP) work, there are certainly many key recommendations within this document that equally apply to numerical models that are used for other types of water resources management solutions (e.g., water quality, floodplain mapping, etc.). For example, the recommendation to store modelling files within a model custodianship program, which will facilitate future use by both consultants and public sector agencies, is universally applicable, regardless of the type of modelling. Since much of the discussion can be extended to modelling outside of the water resources field, practitioners in other applicable fields are also encouraged to make use of this guide.

Examples in this document are most frequently drawn from experience with SWP models and these are typically used for illustrative purposes. The benefit of addressing these types of regional-scale, water budgeting models is that they are data intensive and have significant potential to be adapted for other water management uses, and therefore have a need to be managed continuously.

With the expansion of geospatial data technology, time series analysis, and computational efficiency, numerical modelling is expected to become more prevalent owing to its structured framework, which provides modellers with a powerful ability to interpret large quantities of multi-disciplinary environmental data in support of governance decisions.

1.2 Organisational Structure of Guide

Following Section 1, this guide progresses from high-level to technical-level discussions with respect to modelling and model management. Section 2 serves as a high-level overview of modelling and terminology used in hydrology. It is recommended to all readers, especially for those only loosely involved in model development or management. Here, it is the hope that the reader can gain a very general overview of the model development process.

Section 3 looks at model development in the overall context of policy setting, emphasising the role of models as part of an iterative process that drives the evolution of knowledge infrastructure. This section is again recommended for readers at all technical levels who may be involved in the commissioning and management of numerical models.

Section 4 presents legal and governance issues associated with numerical modelling and is intended for readers directly involved in model development and management.

Section 5 breaks down in detail the requirements and expectations that project managers should consider prior to, during, and subsequent to a model development study. This section speaks directly to those responsible for the management of numerical models. In addition, the section describes, in detail, the data needs that modelling consultants require in order to undertake modelling studies.

Included in the guide are three appendices: i) a glossary of terms; ii) an annotated bibliography for suggested further reading; and iii) a selection of standard contractual templates that are suited to modelling-related Request for Proposals (RFPs) and/or legal contracts, as well as disclaimers for the release of models to third parties.

1.3 BACKGROUND

Through SWP, Ontario has recently embarked on a new era in water resources management, one in which municipalities and conservation authorities have become the recent recipients of numerous technically sophisticated environmental numerical models. As a result of the many technical projects that have been commissioned in the Province of Ontario, mostly under Ontario's Clean Water Act, 2006 (Ontario Legislative Assembly, 2006) but also as a result of requirements under other water-related legislation (e.g., Lake Simcoe Protection Act, 2008 [Ontario Legislative Assembly, 2008], Oak Ridges Moraine Conservation Act, 2001 [Ontario Legislative Assembly, 2001], etc.), municipal government agencies along with conservation authorities now find themselves embarking upon a new pathway for water resources management. This path is one that utilises numerical models as a key tool for understanding and managing water resources in Ontario.

These existing numerical models were built at considerable cost to the public and have resulted in the collection, analysis, and interpretation of data and information, furthering the collective knowledge of the groundwater and hydrological flow systems across broad parts of the province. Given the rapid pace at which the SWP was rolled out across the province, there was little time and effort spent in planning for the longer term management of the numerical models that were prepared under the program. As the technical SWP work wound down, technical staff at municipalities and conservation authorities soon became re-allocated to different programs. As a result, the numerical models are at risk of becoming 'orphaned' in that there is no provincial program in place for their long-term oversight and management. The investment put into these models could be lost.

Although much of the model-related understanding is documented in the many consulting reports that have been issued under the SWP umbrella, it is within the projects' digital files where a significant amount of the work and resulting knowledge has been assembled and synthesised. The longer term management of these digital numerical modelling file packages and the inherent knowledge held within them is the focus of this guide. A model management program will enable the potential future use of these numerical model products, which will help to promote the continual understanding and protection of water resources while leveraging the investments made in the province.

It is worth noting at this point that existing models may not be suitable for application to all future water-related issues. In this regard, checklists for evaluating groundwater flow models for overall soundness can be found in a report by Reilly and Harbaugh (2004) of the United States Geological Survey, *Guidelines for Evaluating Ground-Water Flow Models*. The document is also useful in supporting the review of the applicability of a groundwater model to issues being investigated.

1.4 VISION

Given the movement within Ontario to make use of numerical models through various pieces of legislation, it is worth considering a longer term vision for numerical modelling within the province. In thinking ahead five to ten years, a goal would be to have the following elements of a numerical modelling pathway established across Ontario:

- water resources data will be managed in a comprehensive and integrated manner;
- watershed characterisation, especially information needed to support future modelling exercises, such as subsurface stratigraphy and associated hydraulic properties, land use categorisation (e.g., ecological land classification [ELC], Southern Ontario Land Resource Information System [SOLRIS], etc.), environmental monitoring, digital elevation models, etc., will be accessible at the provincial scale; and
- delineation of hydrologically significant features (e.g., capture zones, significant recharge areas, natural heritage areas, flood hazard zones, etc.) will be derived in a consistent and reproducible manner using numerical models.

Currently, the above activities tend to be undertaken by individual agencies (i.e., municipalities, conservation authorities, etc.). It is envisioned that they could move toward a more collective and efficient approach through partnership arrangements, such as that provided by the Oak Ridges Moraine Groundwater Program (see Section 1.7.3).

Owing to the significant costs associated with modelling, it may prove advantageous to concentrate limited financial and technical resources into several provincially supported 'centres of excellence' to undertake water resources–related numerical modelling activities. In undertaking future modelling studies, such centres, once established, could be destinations where municipal government agencies, conservation authorities, and consultants could turn in order to gain ready access to:

- existing models;
- technical input and guidance from knowledgeable staff;
- model building blocks (i.e., monitoring data, spatial data, stratigraphic layers, land use, etc.) needed to support new numerical models and existing model upgrades; and/or
- a model-related document library.

Considering a province-wide establishment of the above institutions and programs, the following vision is put forward:

> *Integrated water resources management in Ontario will make regular use of numerical modelling tools to inform and enhance water management policy decisions and land use planning. From an established and centralised model management program, models and their supporting data will be made readily accessible to decision-makers through technical staff that have a full appreciation of the models' limitations, range of applicability, and areas for improvement.*

1.5 WHAT IS A MODEL?

A model is simply any device that represents an approximation of a real phenomenon (Anderson and Woessner, 2002). By way of example, consider a toy model train that consists of a locomotive, a series of passenger cars, a caboose, etc. and like an actual train, it will propel along a set track given appropriate fuel. Now, the model train obviously approximates certain features of the real thing (e.g., locomotion along a track, handling of track switches, fuel requirement, etc.) but not others, for example, it cannot actually accommodate passengers or cargo. However, the advantage of the model train is that for those features that the model approximates well, its behaviour can be observed from the safety of a child's bedroom. In broad terms, and for the purposes of this document, a numerical model used in hydrology is a deliberately simplified hypothesis of how the hydrological system works.

Numerical (i.e., mathematical) modelling is no different, but instead of having a miniaturised physical version of the real thing, the physical phenomenon is simulated indirectly by means of governing (mathematical) equations thought to represent the physical processes that occur in reality (Anderson and Woessner, 2002). A numerical model used in hydrology is a deliberately simplified hypothesis of how the hydrological system works (e.g., groundwater and overland flow models). When constructed properly, these models become valuable tools for the management and protection of water resources. In order to construct an appropriate model, adequate field data are required. By using an appropriately constructed model, it is possible to test various management schemes and to predict the outcome of certain actions or policies (e.g., water takings, planned development, etc.).

Once a model has been constructed, realistic answers to meaningful practical problems can be obtained with relatively little effort (as opposed to reconstructing a new model), provided that high quality data in the area of interest are available to constrain the model during development. For this reason, it is worthwhile to properly manage the existing numerical models so that they may be used to inform future decisions. At this time, it is also useful to point out what a numerical model is not: it is not a fact, nor a collection of facts; it is not an oracle to be consulted; and it is not a database. It is a tool that provides the means to use the best available information to help gain an understanding of how the real system works.

1.6 INTRODUCTION TO MODEL MANAGEMENT

The development of numerical models involves many technical tasks: i) project scoping, ii) data collection, analysis, and interpretation, iii) developing a conceptual understanding of the real-world system and other relevant processes, iv) capturing all of this into a numerical simulation of the system, and v) reporting on the model results. Such activities are costly, however, they can be thought of as a knowledge infrastructure, which can and should be utilised long into the future. It is argued here that numerical models and the knowledge infrastructure they provide are of sufficient importance that they should be managed in a similar manner to ordinary hard infrastructure (e.g., pipes, roads, power supply, treatment plants, etc.). Thus model-based knowledge infrastructure should be considered a public asset and should be built into an agency's asset management plan. As required with hard assets, all of the components of a numerical model require ongoing maintenance, management, and upgrades.

Numerical model management can be considered to be the procedures an organisation must take to maintain model-related knowledge and data, as well as the actual models themselves (i.e., digital files), for future distribution and application. Any agency that commissions numerical modelling studies does model management – either implicitly and unintentionally, or explicitly and with specific management goals and future planning. Model management includes procedures for (adapted from Arnold, 2013):

- collecting, analysing, and organising necessary data;
- sharing of input and output data;
- communicating processes, applicability, interpretation, and results;
- storing/archiving digital files;
- translating direct model outputs into results for evaluation;
- updating or repurposing models for future use, including for uses outside of the original design intentions; and
- terminating models when deemed necessary, such as when new models or technology emerge.

The goal of model management is to optimise the utility derived and information gained from a modelling exercise by considering all associated short- and long-term costs and benefits. Benefits of modelling not only include the information and knowledge obtained during the model's development, but the ability to review and utilise data collected from various monitoring programs for the purposes of supporting current and long-term decision-making and environmental planning. Costs are initially associated with consultants hired to build the model and are subsequently linked with internal staff (or consultants) tasked with the agency's future use of the model (e.g., rerunning the model, training costs, software fees, data management, hardware upkeep, etc.).

1.7 Ontario's Path to Numerical Modelling

Starting in 1998, the Province of Ontario launched a Groundwater Management Studies program (GMSP), which was mostly funded by the Province (up to 85%). These studies were designed to help characterise surface water flow systems and the subsurface environment both from a geological and hydrogeological perspective. Following the Walkerton tragedy of 2000, there was an onset of comprehensive work designed to start-up a SWP program. In ideal cases, the information from the GMSP formed part of the baseline information that was incorporated into the more recent SWP work. In such cases, the early characterisation work has become less significant as new SWP work largely incorporated and built upon the older work. In other cases, earlier work was replicated rather than built upon, resulting in multiple but perhaps equally valid interpretations.

More recently, concurrent with and following on the SWP program, other provincial programs and/or pieces of legislation (e.g., Lake Simcoe Protection Plan [Ontario Legislative Assembly, 2008]) have in some cases also led to improvements or refinements of earlier SWP subsurface characterisations, as well as to the development of additional, and in cases overlapping, numerical models. In all cases of either overlapping models or newer models replacing older models, it must be noted that the end result is that different interpretations and model results can arise, and also that these differences may have been founded on differing data sets. All of this must also be considered as part of Ontario's future model management strategy.

It is worthwhile to take a look at existing situations at local agencies that are engaged to some degree in longer term numerical model management. First, experience from York Region is instrumental in demonstrating the need for model management in larger government organisations, in order to keep track of how models are used and what changes are incorporated as different staff and departments take a numerical model, alter it, and use it for different purposes. Next, a case study from the Grand River exemplifies where one model has been re-used and updated over time to continually provide meaningful input to decision-making within the watershed. Lastly, the Oak Ridges Moraine example provides a case study where many agencies have banded together for groundwater management purposes to better capitalise on limited financial and technical resources.

1.7.1 Case Study – Regional Municipality of York

York Region was provided funding in 2001 and 2002 by the Ontario Ministry of the Environment to improve its understanding of the groundwater flow system and the sustainability of its water supply, particularly to the Newmarket and Aurora communities. Under the direction of its Water Resources group, the Region joined with adjacent agencies (Peel, Durham, and Toronto) to jointly commission a comprehensive numerical modelling study that covered a large geographical area stretching northwards from Lake Ontario in the south, across the Oak Ridges Moraine to the Lake Simcoe area in the north. The end product was a comprehensive, steady state, numerical model that reasonably reflected the geological layering and observed groundwater conditions across the area. The model was informally termed the Core Model.

Model management challenges arose over the four years during which the Core Model was being built. While the consultant was still engaged with the model work, environmental assessment (EA) studies were underway to support a number of construction projects situated within the boundaries of the regional-scale Core Model. Since the model was largely complete, although not yet finalized, a decision was made to utilize the Core Model for supporting these various construction projects. The result was that the initial Core Model was altered on a localised basis prior to its finalisation and the delivery of the digital files and supporting documentation. In part due to capital project schedules, but also because model management processes did not exist at the time, these localized adjustments were not re-incorporated back into the initial Core Model. This left York Region and the ORMGP with multiple model versions, as opposed to a single, continually refined, authoritative product.

Not long after the delivery of the Core Model, additional provincial funding through SWP was made available to assess water quantity risk to current and future municipal drinking water sources under a number of scenarios (e.g., growth, drought, etc.). The original Core Model was updated and refined to become the York Tier 3 model. The process involved converting the steady-state Core Model into a transient, integrated groundwater/overland flow model. Although the York Tier 3 model did consider and incorporate work that was undertaken subsequent to the Core Model completion, the conceptual, structural, parametric, and boundary condition differences between the Core Model and the York Tier 3 model were not fully documented.

York Region, with the assistance of the ORMGP, is working to ensure the Tier 3 model remains up-to-date and is the authoritative model for water resource management decisions. This task could have been avoided or at least minimized, with more rigorous contract preparation, better communication, and clearer processes for model management. Going forward, York Region, again working with the ORMGP, have processes in place to capture model refinement efforts through regional or partner-led consulting assignments. York Region's consulting contracts now require that model refinements are returned to the Region, along with appropriate documentation and digital files. This will help ensure that the Tier 3 model remains the authoritative model for water resources management decisions.

1.7.2 Case Study – Grand River Simulation Model

In order to evaluate strategies to control eutrophication within the Grand River, the Grand River Simulation Model (GRSM) was built by the Ontario Ministry of the Environment (MOE) and the Grand River Conservation Authority (GRCA) in the 1970s. It built upon similar work that had been done in southwestern Ontario, where a dynamic simulation model was used for the same purposes in the Thames River. In 1982, the model was used to evaluate water management options for the Grand River Basin Water Management Study. The GRSM remained unused for a number of years, until the issue of increased wastewater treatment plant discharges in Waterloo and Guelph (as a result of increasing urban development) was raised in the early 1990s. At this time, the model underwent a major upgrade to overcome hardware and software limitations resulting in more streamlined input and output processes. The equations describing plant growth and inhibition were reviewed and revised as needed to remain consistent with ongoing research. As part of the Middle-Grand River Assimilative Capacity Study completed in 2010, ammonia volatilisation and denitrification were incorporated into the GRSM to provide a more comprehensive picture of important nitrogen cycle processes occurring in the Grand River. The GRSM focussed on dissolved oxygen (DO) as the most important indicator of river water quality since DO levels play a large role in determining the level of stress on fish communities and diversity of the fishery in the river. With further updates over the years, the model can now also be used to evaluate biochemical oxygen demand, nitrogenous oxygen demand, and nitrate, suspended solids, and total phosphorus concentrations.

The improvements and modifications that have been made to the GRSM provide a concrete example of how modelling and effective model management and documentation of model changes can be used in Ontario to inform decision-making. The GRSM is freely available through the GRCA, and scientists, engineers, and planning staff make use of the results to understand how proposed land use changes within the watershed might affect the quality of water in the Grand River.

1.7.3 Case Study – Oak Ridges Moraine Groundwater Program

Throughout the 1980s and 1990s, development was encroaching upon the Oak Ridges Moraine in central Ontario and threats to groundwater resources were of great concern to local residents. Municipalities and conservation authorities repeatedly turned to the Province requesting that the issue be addressed. With little to show in terms of provincial implementation, in the late 1990s, the Regional Municipalities of York, Peel, and Durham banded together, and were later joined by the City of Toronto (forming YPDT), to better address groundwater management with a focus on the Oak Ridges Moraine and the watersheds draining from its north and south flanks. At the same time, conservation authorities were similarly concerned with the Oak Ridges Moraine's groundwater and formed a coalition of the nine conservation authorities having jurisdiction on the moraine (Conservation Authorities Moraine Coalition [CAMC]). The coalition recognised deficiencies in their groundwater management activities and was determined to contribute to an improved approach.

These two initiatives (YPDT-CAMC) led to the formation of the Oak Ridges Moraine Groundwater Program (ORMGP) and the hiring of a program manager in 2001 to better coordinate groundwater management across a broad part of central Ontario. Since this time, the program has grown to become a focussed centre of excellence for groundwater management and provides a concrete example of how groundwater information and knowledge can be more effectively managed within the province. The program initially focussed on groundwater data management and then strategically moved to build on earlier work by the Geological Survey of Canada (GSC) to establish an authoritative regional geological framework into which other studies could be set. The program also initiated and oversaw the creation of several numerical groundwater models, including the Core Model along with York Region. This initiative predated the initiation of the technical SWP work, which began in 2008.

More recently, the program has boosted numerical modelling expertise by hiring a modelling expert, thus establishing the program as a logical vehicle for numerical model management within central Ontario. Currently program staff have reviewed and commented upon over 50 regional-scale numerical models that have been developed over the past decade. Several modelling software packages have been acquired to facilitate the review of the models and they have all been run to completion, thus ensuring that the file delivery has been successful and that there are no missing or corrupt files. The models are now archived and are available to the partner agencies should they be needed in the future.

The ORMGP serves as an example of how multiple agencies can collaborate to establish a program specific to the handling of technical data and numerical modelling products. Having this knowledge infrastructure within a centralised institution has greatly improved the efficiency with which its partners can access the water resources data necessary for decision-making and planning in a timely manner. Experience gained from the management of numerical models, an ongoing activity within the overall ORMGP, has had much influence upon the development of this guide.

1.8 Collaborative Modelling Approach

Experience has shown, both within and outside SWP modelling studies, that the best modelling experience, from the perspective of both the public sector agency and the consultant, occurs when both parties are actively engaged throughout the model building process. Given that modelling is technically sophisticated and is typically an iterative process, the knowledge gained from the collection, analysis, and synthesis of data used to build a model is best developed through a collaborative effort. While maintaining an active client–consultant collaborative relationship during a model building project can be time consuming and costly, it nonetheless provides a pathway of effective knowledge infrastructure growth. It should be pointed out here that collaboration does not necessarily mean meetings. Certainly some formal meetings are required over the course of any given modelling project, however,

EXAMPLES FROM EUROPE – POSSIBLE PATHS TO FOLLOW?

Denmark perhaps sets the bar in terms of maintaining, managing, and updating complex watershed system models, which are used as tools to assist in water resources decision-making. In 2003, the Geological Survey of Denmark and Greenland developed a national-scale water resources model for Denmark that is a "mechanistically, transient and spatially distributed groundwater-surface water model" (http://vandmodel.dk), using the MIKE SHE/MIKE 11 (http://www.mikepoweredbydhi.com) model code.

Similar to many democratic countries, Denmark has three tiers of government (national, state, municipality) and each level has a technical staff with sound modelling knowledge who receive regular technical training as well as education on Denmark's national modelling guidelines. With increasingly detailed local knowledge being available, the need to incorporate local conceptualisation into the national model became apparent since the national model was being used to provide boundary conditions and other key insights for local assessment models. Making use of technical staff at all three levels, an update process was initiated that focussed on: i) basic data (e.g., time series); ii) details in the model description (finer discretisation); and iii) improvement in model processes. All stakeholders provided input into strategic elements such as determining the model updating frequency, how to integrate local knowledge, and determining future model uses and requirements. Key challenges included: i) working with both groundwater and surface water departments in order to integrate data at national scale; ii) agreeing to consistent data handling; iii) establishing processes to effectively integrate local/regional models with the national model; and iv) keeping costs from escalating.

Shared software tools play a pivotal role in Denmark's model management system. These include central data storage, tools for interpolation of model grids, data correction, and data visualisation, as well as preprocessing tools. Capacity to use these tools was built across all agencies through workshops and conferences. The polycentric government system also posed challenges with respect to financing, distributed responsibility, differing timelines, capacity building at lower tiers, and meaningful involvement of higher level stakeholders. Key elements of this successful model management strategy include: i) continuous access to knowledge and staff resources; ii) mechanisms to transfer knowledge between different disciplines and levels of government; iii) knowledge sharing; and iv) meaningful engagement of the modelling community.

A similar path was followed in the Netherlands, when in 2005, with an annual budget of 1 million euros, regional water authorities pooled expertise and started building a national-scale model and toolkit (now referred to as the National Hydrological Instrument [NHI]). The NHI established a free data management gateway providing access to national and regional databases as well as model input and output data. The government also invested in converting model codes, workflow management, and processing tools into open source software, much of which is now accessible at no charge through their OpenEarth gateway (http://www.openearth.nl). By 2013, virtually all water management organisations of the country were using this tool. The NHI connects all water domains with five linked models: saturated groundwater, overland flow, soil-vegetation-atmosphere transfer, hydrodynamic flow and transport in larger water bodies, and, finally, a water allocation tool. Recently, the NHI has moved to an open approach to addressing intellectual property rights by promoting crowd-sourcing for innovation. Today, the NHI provides boundary conditions to regional models and is used for complex analyses like saltwater intrusion, cost-benefit analysis for water allocation, nutrient leaching, and pesticide management.

Although not as comprehensive as the Denmark and Netherlands examples, the United Kingdom has also developed considerable modelling expertise, with a focus on groundwater modelling. Starting in the early 2000s, England and Wales embarked on a program of numerical groundwater modelling to improve the understanding of water resources. Using technical consulting firms, regional-scale models were constructed across England and Wales. To facilitate the access and running of the models, the National Groundwater Modelling System was established to host the models online. Using 'model adapter' software developed by Deltares (http://www.deltares.nl), the adapted MODFLOW (a United States Geological Survey model [http://water.usgs.gov/ogw/modflow]) models are available online, allowing users to run 'what-if' scenarios. Besides pumping schedules, no other model changes are permitted, however, the models are updated on an as-needed basis.

collaboration in this section refers to working meetings where there is no expectation of formal presentations, but rather simply a productive exchange of knowledge as various modelling activities are being worked upon. Active technical engagement from both the client and the consultant results in: i) the development of numerical models that better reflect a shared conceptual understanding; and ii) a model design that is optimally suited to address the agency's water resources–related issues. There are several key benefits that a collaborative approach provides:

- from the public sector agency client perspective:
    - it allows staff to gain an appreciation of the amount of work needed to build and run a model;
    - it allows staff to become familiar with the model's applicability and limitations, and perhaps become sufficiently trained to run the model for internal use;
    - it can provide staff with greater insight into the quality of their monitoring data;
    - it permits staff to better understand how the physical system might be working when they are allowed to see watershed responses to various input stresses; and
    - it provides staff with the confidence to speak intelligibly on the model results and insights gained from the model;
- from the consultant perspective:
    - it provides consulting staff with intricate watershed knowledge (e.g., certain streams are dry in late summer months, residents have complained in this area about wells drying up, etc.) that can assist with model development and calibration thereby allowing parameters to be more readily adjusted to better reflect system behaviours;
    - it can help clarify the needs of the modelling study to prevent the study from going off track; and
    - it allows consulting staff to better understand the overall physical system and to focus on the computer and numerical aspects of the modelling process by making use of the client knowledge and expertise for background knowledge in how the watershed functions.

2 MODELLING FUNDAMENTALS

This section presents a high-level overview of watershed modelling for the purposes of managing water quantity. It is presented as a non-technical overview of modelling processes and provides common terminology, with which managers, especially those with little modelling experience, must become familiar. The discussion draws almost exclusively from the experience of the source water protection (SWP) program and may not necessarily speak to all practical disciplines of numerical modelling. The intent of this section is to only serve as an introduction to numerical modelling applied in watershed management and for more detailed information the reader is directed to the annotated bibliography (Appendix 2), which provides additional references for technical support.

Numerical models are built to help formulate professional opinion and support decision-making in situations involving complex information and processes. Modelling offers a multitude of approaches for integrating scientific knowledge and observed monitoring data into a singular framework, enabling the translation of a conceptualised system into a logical framework (i.e., computer code). Once completed, models not only provide predictions that assist in answering questions, but, as they are built, they contribute to the understanding of the real system, at times in surprising and unexpected ways. Models have the power to incorporate many disparate data, and provide a powerful means of detecting poor quality data that could otherwise be overlooked. Models can also help to identify optimal areas where data gaps need to be filled. It is anticipated that modelling will emerge as an iterative process, with key models continually evolving, benefitting from, and contributing to, an increasing understanding of real-world systems.

For the purposes of this guide, a watershed model reflects any numerical model used in hydrology that was built to estimate water quantity and quality at the *watershed scale*, such as the many models built under the SWP. Watershed-scale models will likely require long-term management as they are generally intended for continued use by public sector agencies.

2.1 TERMINOLOGY

It is important to appreciate that terminology used in hydrology can vary between different subdisciplines of hydrology. This poses linguistic challenges for modellers and model managers. For example, groundwater modellers use the term ‘surface water model’ broadly to incorporate any model that simulates surficial processes, including both hydrological models (e.g., Precipitation Runoff Modeling System [PRMS], Hydrological Simulation Program – Fortran [HSP-F], Hydrologic Modeling System [HEC-HMS], Guelph All-Weather Storm-Event Runoff [GAWSER], etc.) and hydraulic models (e.g., Hydrologic Engineering Center River Analysis System [HEC-RAS], Stormwater Management Model [SWMM], MIKE 11, etc.); in contrast, flood hazard analysis engineers use the term surface water model to specifically refer to shallow-water hydraulic models (e.g., HEC-RAS, SWMM, MIKE 21, etc.). There is an important distinction between hydrological and hydraulic models. A hydrological model refers specifically to water balance models that account for the quantity of water in space and time (i.e., conservation of mass); whereas a hydraulic model must also account for the movement of water in space and time (i.e., conservation of momentum). While hydraulic models tend to involve more sophisticated mathematics, most hydraulic modelling solutions ultimately depend on a hydrological simulation.

As a further example, the term ‘infiltration’ is often used in hydrology to describe the pathways from which water is being added to the system being modelled, and is thus dependent on the perspective. Municipal engineers would view infiltration into storm sewers as a *loss* from the groundwater system; whereas hydrogeologists would view infiltration as a *gain* to the groundwater system. This obvious contradiction in view shows how model management can become unduly convoluted.

Throughout this guide, such terminology differences are highlighted, however, there is no intention here to prescribe or redefine terminology. Rather, the intent is to rely on consistent terminology for the purposes of discussing watershed-scale model management. Some modellers will find that the language used in this guide may be slightly different than the language used in their subdiscipline and experience. Model managers must be aware of this linguistic confusion, especially as integrated modelling approaches become more prevalent.

2.1.1 The Hydrological Cycle

The hydrological cycle describes the flow of water through the environment (Figure 2-1). Water travels through the atmosphere as vapour or clouds, precipitates to the Earth’s surface as rainfall or snow, is intercepted at the vegetation or leaf litter layer where it trickles as throughfall and stemflow to the soil surface. There, the water infiltrates into the soil, evaporates back into the atmosphere, or runs off. Runoff can then infiltrate into the ground elsewhere, get collected in ponds or other puddles, or supply creeks and rivers. Water that has infiltrated into the soil zone may be absorbed by plants and transpire back to the atmosphere, directly evaporate (if near the surface), or percolate down towards the water table to become groundwater recharge. Once in the groundwater system, water will move slowly, eventually discharging to seeps, springs, streams, wetlands, rivers, lakes, and oceans, or it will remain trapped for geological-scale time periods in stagnant zones. The term ‘hydrological system’ or ‘system’, as used below, describes the environment through which water flows.

Physically accounting for water quality and quantity at any particular time or location can be accomplished in principle, but in reality this is practically infeasible; a more cost-effective approach is to collect all available data and develop a numerical model. Numerical models are used in hydrology to simulate all aspects of the hydrological cycle shown in Figure 2-1, in particular, the movement, distribution, and quality of water. These models are built to provide an understanding of one or more processes involved in the hydrological cycle, including:

- Precipitation, which falls as either snow or rainfall, and is the main source of water to the system. System behaviour is ultimately dependent on the amount of precipitation delivered over the time period of interest.

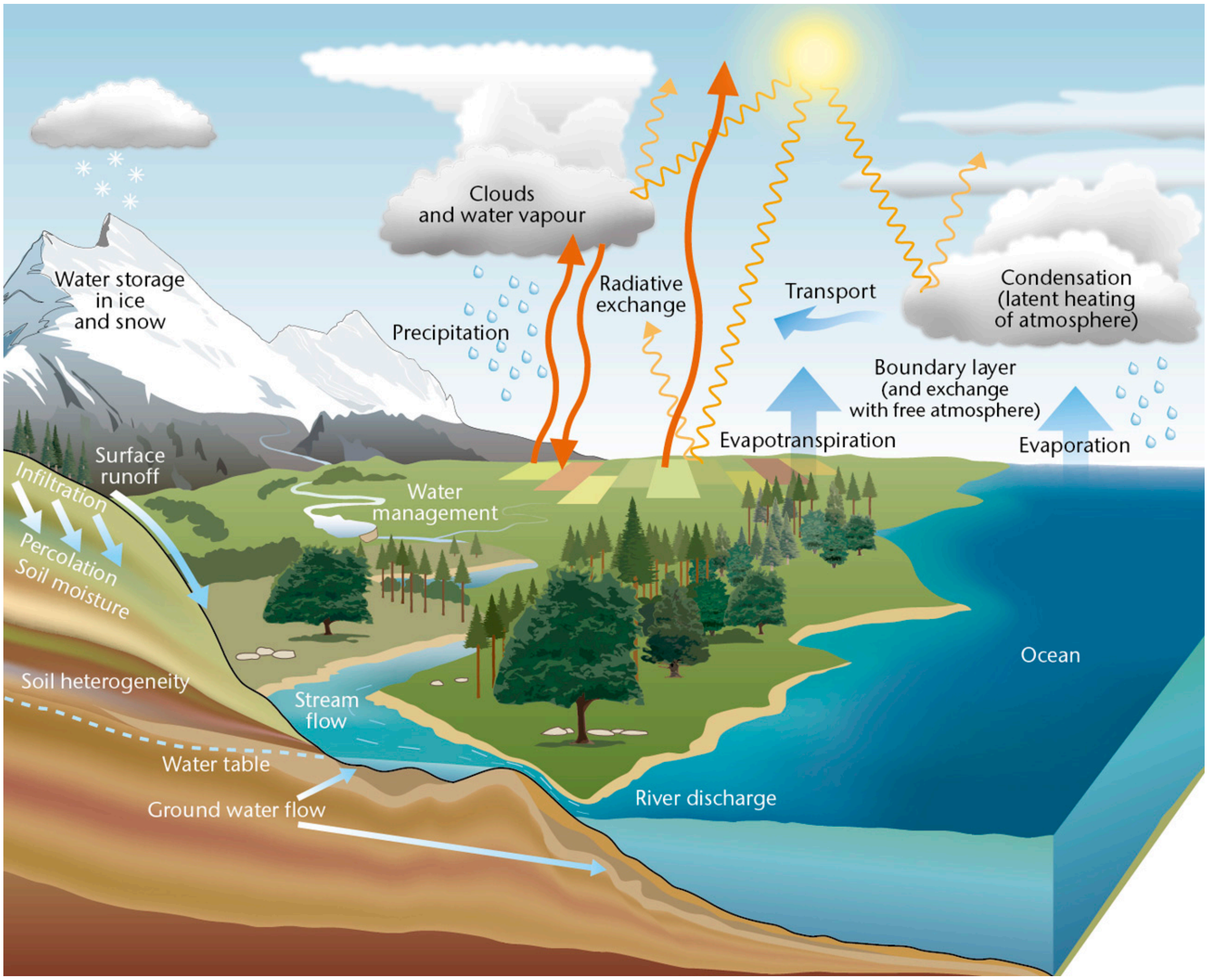


Figure 2-1: Conceptual diagram of the hydrological cycle and its various pathways (Met Office, 2017, contains public section information licensed under the Open Government Licence v1.0).

- Interception, which is precipitation that does not immediately reach the soil because it is intercepted either by canopy leaves and branches, or at the forest floor by the leaf litter layer and short vegetation.
- Infiltration, which is precipitation that reaches the ground surface and is absorbed by the underlying soil. This water can either be lost to evapotranspiration or can move downwards to recharge the groundwater system.
- Evapotranspiration, which consists of both the abiotic and biotic processes involved in the loss of water from the earth's surface to the atmosphere. In general, evaporation occurs where water is exposed to the atmosphere, whereas transpiration is the biophysical process of water movement through vegetation and subsequently to the atmosphere.
- Radiative exchange, energy that originates from the sun that drives evapotranspiration and warms the atmosphere.
- Runoff, which is generated in areas where rainfall exceeds the capacity with which water can infiltrate the soil; excess water will pool and/or contribute to overland flow.

- Overland flow, which represents water that travels laterally across the landscape, generally in a downslope direction.
- Runon, which results from overland flow occurring in upslope areas and arriving in downslope areas. This runon may then infiltrate at this downslope location or contribute to runoff if the infiltration capacity is met.
- Groundwater recharge, water that infiltrates the near-surface soil horizon and percolates downward eventually reaching the groundwater table and recharging the groundwater supply.
- Groundwater discharge, which occurs when groundwater rises above the land surface, results in water seeping above-ground or directly into water bodies.
- Groundwater flow, water that is present within subsurface pore spaces moving along a falling energy gradient.

The above description reveals another set of apparently ambiguous terms: runoff, runon, and overland flow[1] are commonly used interchangeably depending on which modeller and/or model is being used. For example, models used in a rainfall-runoff simulation do not explicitly account for the spatial movement of water, therefore overland flow and runoff become synonymous and runon has no meaning. Differentiation of these terms becomes important for models that simulate distributed processes (e.g., where the conveyance of water through the landscape is accounted for), which is the case for the models built for SWP and that are the focus of this guide.

The remainder of this guide focuses on quantitative aspects of modelling the hydrological cycle at a watershed scale, and therefore does not include matters related to water quality modelling. It should be noted, however, that the understanding of the distribution and quantity of water within the hydrological system is paramount in the prediction of water quality. Many other common applications of numerical models used in hydrology are omitted from this guide, especially those that are context- or project-specific or at a small spatial scale (e.g., lot level).

2.1.2 The Suite of Modelling Tools Used in Hydrology

Water quantity hydrological models are the most likely to assist in future water management–related decisions and require continual management by public agencies. Table 2-1 outlines the various types of hydrological models used to investigate watershed-scale processes. The table highlights the processes they simulate and their typical data requirements. The model types have been defined/grouped based on attributes that relate to their relative complexity and data needs:

- dimensionality relates to the complexity with which the numerical model is simulating real-world hydrological *processes* and is directly proportional to data needs, model complexity, modeller specialisation, model cost, model run-times, etc.;
- spatial resolution relates to the degree of simplification used to represent the watershed *system* and is generally correlated with dimensionality; and
- scale refers to the geographical extent to which the models are applied.

[1] Other terms include sheetflow, surface water runoff, surface runoff, etc.

Table 2-1: Characteristics of environmental model types used in watershed-scale hydrological models.

Model type	Phenomena/ simulation	Dimen-sionality	Spatial resolution	Scale	Data needs
Flood forecasting, rainfall-runoff, lumped parameter, semi-distributed	flow frequency analysis: recurrence, peak, magnitude, duration; hydrographs	0D	very coarse	subcatchment to watershed	precipitation, streamflow
River hydraulics	flow depths, shear stress and erosion, transport, habitat	1D	coarse	reach to watershed	streamflow, channel survey, topography
Hydrological, water balance	water balance, water cycle (i.e., runoff, recharge, evapotranspiration, snowmelt)	2D	fine to coarse	site to watershed to continent	meteorological data (precipitation, rainfall, snowfall, temperature), potential evapotranspiration, streamflow data, land use, regional physiography, topography
2D hydraulic, hydrodynamic, shallow water, surface water, fully distributed	contaminant transport, shear stress, sedimentation, flow depths and velocities, flood extents, habitat, life safety/emergency planning, spill flow	2D	fine	reach, floodplain, urban centres	topography, land use planning, channel survey, design storms/hydrographs
Groundwater modelling	groundwater levels, drawdowns, contaminant transport, seepage, baseflow	2D–3D	fine	site to watershed to continent	hydrostratigraphy, groundwater monitoring and pumping info, recharge, lake water levels
3D hydrodynamic	currents and tides, contaminant transport, sedimentation, coastal zone management, marine management	2D–3D	fine	water bodies (lakes, oceans, large rivers, estuaries), marinas	bathymetry, coastline delineation, lake water levels, wind speeds, currents, river discharge

Each model type listed in Table 2-1 poses unique challenges and solution strategies. For example, flood forecasting models predict the frequency, duration, and magnitude of flooding at one or more points typically with assumptions of homogenous land use and climate (i.e., imperviousness of surfaces and antecedent conditions); these models can offer great utility and rely solely on rainfall and streamflow data. On the other hand, regional groundwater models are required to predict water distribution in three-dimensions varying with time. Thus a greater variety of data is required in order to characterise subsurface aquifer and aquitard systems.

Another example is one-dimensional hydraulic models that are used to determine how flood waves move along a channel and estimate their impact on manmade structures and predict erosion to channel bottom and banks. However, these models simplify the riverine flow system to a one-dimensional process and disregard much of the spatial detail necessary for a watershed-scale model. Ultimately, the choice of a model and the associated data requirement depends on the problem that needs to be addressed as well as the scale of the study.

The dimensionality aspect of models, as presented in Table 2-1, provides a good rule-of-thumb that a model manager can use to gauge the sophistication of anticipated modelling projects. Zero-dimensional or lumped-parameter models offer the simplest and most efficient modelling solutions, however, they tend to be limited to specific applications and are restricted to a single point in space. As dimensions are added, an exponential increase in information is required to build the model. The effort and time required also increases significantly.

Much literature exists for the model types listed in Table 2-1. For further details on zero-dimensional (0D) or lumped-parameter watershed models (first row in Table 2-1) see Harter and Hopmans (2004), Pender (2006) and Woodhead et al. (2007). Xue et al. (1991) documents 0D (lumped-parameter) models used in climate modelling and Singh (2012) provides detailed descriptions of a multitude of watershed models used in hydrology, most of which fall in the lumped-parameter rainfall-runoff category. Beven (2012) also provides a thorough discussion of lumped modelling and its implication.

One-dimensional channel modelling (second row in Table 2-1) is also well documented, with Chow (1959) providing the benchmark reference on open channel flow. Ponce (1989) provides sound theoretical detail on the numerical implementation of 1D models, whereas Julien (2002) provides a broader perspective of channel flow, focussing on sedimentation and fluvial morphology.

Two-dimensional modelling of shallow water equations (fourth row in Table 2-1) has been much discussed in journals, but outside of academia, resources are lacking, likely due to the increase in sophistication. A recent reference, Di Baldassarre (2012), provides a wealth of pertinent references and presents a concise overview of theory and recent advances and applications.

Three-dimensional groundwater modelling (fifth row in Table 2-1) has a wealth of references, some key ones are Spitz and Moreno (1996), Willing (2007), and Anderson et al. (2015).

Three-dimensional hydrodynamic modelling (sixth row in Table 2-1) is the most technical of the presented model types. A recent publication on 3D hydrodynamic models with an environmental focus can be found in Bates et al. (2005).

This leaves spatially distributed two-dimensional (2D) hydrological water-balance modelling (third row in Table 2-1; the focus of this guide). Unfortunately, there are few references on distributed models to turn to for direction. Until recently, all watershed modelling would have either been accomplished using zero-dimensional or semi-distributed models (see discussion on distributed modelling in Section 2.2.2).

Early publications on distributed modelling in hydrology include Abbot and Refsgaard (1996) and Grayson and Blöschl (2000). At the time of these publications, computational capabilities were limited for practical modelling application and, consequently, few resources outside of academia were directed to this line of modelling. Under the SWP program, especially with respect to groundwater resources, an important requirement of hydrological modelling was that the models provide a determination of the groundwater recharge distribution across much of southern Ontario, a geography characterised by a diversity of surficial geology landforms and materials. Healy (2010) recently published a textbook on recharge estimation that highlights the distributed nature of the recharge-related processes, especially in geologically heterogeneous landscapes, as typified by southern Ontario. Although Healy includes some discussion on modelling, the text mainly focusses on physical methods for recharge estimation.

The lack of literature on watershed- or regional-scale, process-based, distributed modelling poses a challenge for those managing SWP models. In addition, the current state of computation technology has allowed for the emergence of integrated groundwater/surface water modelling, combining nearly all model types listed in Table 2-1. The SWP hydrological and integrated models were built to cover large watershed-wide areas, but with a fine spatial discretisation in order to distribute the hydrological processes more discretely. As a result, SWP watershed models were pushed beyond the standard practice and available literature.

2.2 REGIONAL-SCALE HYDROLOGICAL MODELLING

Distributed watershed-scale hydrological modelling for the purposes of regional water budgeting inherently requires the incorporation of multiple fields of discipline, such as meteorology, physiography, river mechanics, plant physiology, ecology, hydrogeology, etc. From a numerical modelling context, many of these fields interact at the water-soil-vegetation-atmosphere interface and must coherently fit together across vastly different spatial and temporal scales.

Naturally, this is a conceptual challenge affected by technical difficulties such as the sheer number of different data sources required, the resolution and quality of the data, the variability of a model's spatial and temporal resolution, all coupled with the complexity of feedback mechanisms. Modern watershed models offer several options to handle each physical process through individual computational modules, however, each module represents a specialised field of knowledge with its own subdisciplinary lingo.

Furthermore, distributed regional-scale watershed modelling is less standardised than the individual model types listed in Table 2-1. A likely reason is that many model codes are built to fulfil a specific set of objectives focussing on one specific process of the hydrological cycle. This allows modellers to simplify or even neglect other hydrological processes that are less relevant. For example, flood forecasting focuses on runoff during high water conditions, whereas baseflow is less important. Total upstream water retention is relevant, but it is less important to exactly understand whether this retention is caused by infiltration, ponding, or plant interception. A simple (a.k.a., parsimonious) model will very accurately simulate runoff and routing in creeks, but offer only a crude approximation as to the runoff generation mechanisms. Similarly, in assessing low flow or drought conditions in Ontario streams, the most important processes may be groundwater discharge to the watercourses (i.e., baseflow) and water takings. An appropriate model would need to simulate groundwater flow and discharges into the river as well as river routing, whereas overland runoff contributions could be simplified or neglected entirely. These simplifications are advantageous, as data needs can be greatly reduced and background knowledge and experience can be narrowed. As a result, application of these process-specific models proliferated and inevitably became the established standard.

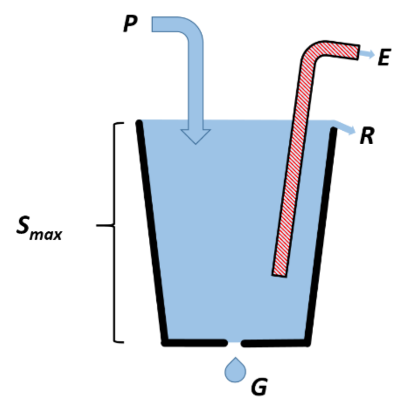
2.2.1 Integration of Groundwater and Surface Water

In Ontario and abroad, the need for a proactive assessment of watershed health has become an increased concern in the field of watershed hydrology. Because the various indicators of watershed health (e.g., wetlands, coldwater streams, habitats, etc.) tend to be associated with the water-soil-vegetation-atmosphere interface, the need to simultaneously simulate the interactions of the various phenomena listed in Table 2-1 has become essential. As a result, the simplification of certain hydrological phenomena for the sake of addressing specific objectives is proving less effective in addressing many societal concerns and can no longer be relied upon. This has led to greater complexity in model conceptualisation, which requires innovative approaches with few standardised methodologies to draw from. A comprehensive form of modelling, loosely termed integrated modelling, represents the attempt to unify all (or most) of the hydrological processes into one modelling platform.

The integration of the many subdisciplines of hydrology presents a challenge with respect to unifying terminology. When hydrological processes are modelled separately, terminology is often used in differing and ambiguous ways. Naturally, as the development and application of integrated models increases, these ambiguities will need to be resolved. Terms are used consistently throughout this guide.

2.2.2 Lumped versus Distributed Modelling

A significant source of ambiguity arises from the concepts of lumped versus distributed modelling. Although the application of these terms is somewhat controversial amongst some modellers, they simply refer to the spatial discretisation within the model. The simplest hydrological model is a zero-dimensional rainfall-runoff model, commonly known as a lumped model (Xue et al., 1991; Harter and Hopmans, 2004). Lumped models (or lumped-parameter or lumped-variable models) have been conceptualised very effectively using the 'bucket' analogy (Manabe et al., 1981); the inset box on this page explores this analogy by use of a cup instead of a bucket. What the



Consider a conceptual cup with a finite storage capacity. Once its capacity is exceeded, it will spill over. This cup is poorly fabricated and slowly leaks through its bottom. Assume, too, that an arbitrary amount of water pours into the cup and water can be simultaneously extracted from the cup by sucking water through a straw. As simple as this is, it is all one needs to know about how rainfall-runoff models work.

In this analogy, the cup represents storage at the land surface (neglecting for the moment storage associated with vegetation). Like the cup, the soil zone has a storage capacity (S_{max}) and once that capacity is exceeded, runoff (R) is produced. Like the water leaking from the cup, water stored in the soil zone will percolate/drain downward (G). Due to atmospheric conditions, some of the stored water will be removed by evapotranspiration (E). Finally, the soil is replenished periodically by precipitation and snowmelt events (P).

bucket represents in terms of hydrological modelling is a computational unit, that is, a numerical representation of some representative elementary volume, where sources and sinks are accounted for and mass and energy is conserved. It follows that in a lumped model all of the hydrological processes that occur within a watershed are spatially averaged; meaning that the entire watershed has been treated as a single computational unit.

A watershed contributes runoff to a particular point in space, for example, where a river crosses underneath a bridge, thus one can roughly assume that all the water flowing beneath a bridge was at one time water that precipitated within its watershed. Lumping a watershed into one computational unit is extremely effective for predicting stream flow rates. However, in lumping watershed processes, there would be absolutely no context as to what parts of the watershed contributed the runoff, or where infiltration was the greatest. Terms like runon would have no meaning, and groundwater recharge and discharge could not be differentiated. Aggregated parameters, like net recharge, would then be required. Groundwater flow, being inherently a spatial phenomenon, would necessarily have to be neglected or greatly simplified. However, if it is possible for the modeller to neglect these processes (i.e., they are unimportant to resolving the issue at hand), then a lumped model would be a highly effective and logical approach, as the model is simple to develop and generally has fewer data requirements.

Lumped models need to be restricted to small-scale watersheds (<100 km^2) for the simple fact that weather patterns (i.e., precipitation, temperature) tend to vary spatially at larger scales. In addition, this approach is limited to simulating watershed response only at the mouth of the watershed (or to follow the example above, water under the bridge). A simple solution then is to break-up the watershed into many smaller logical subwatersheds. Consider the schematic of a watershed shown in Figure 2-2a. With a lumped model, all of the five wetlands, every stream reach, and everything in between would be represented by a <u>single</u> computational unit (c.f., cup). In order to attain a level of spatial heterogeneity, the watershed could be subdivided into a number of subwatersheds, logically divided according to the location of tributaries and stream reaches (Figure 2-2b), each now their own computational unit. Traditionally, this process of watershed subdivision is defined as distributed modelling.

However, to a degree, this watershed conceptualisation remains lumped: it now describes the system as a set of lumped models operating in series and parallel in some topological context. For example, the watershed shown in Figure 2-2b can be equally represented graphically as Figure 2-2c, where each number (subwatershed) is being simulated by an independent lumped model.

It is important to point out that for this conceptualisation, the model is commonly considered distributed, but only in terms of the model forcings (i.e., the input variables that drive the model, such as precipitation, temperature, etc.); however, the processes that occur within each subwatershed have no influence on adjacent subwatersheds. It is best to consider this conceptualisation as *semi*-distributed. Therefore the limitations with lumped models, as noted above (i.e., runon, groundwater discharge, recharge, etc.), persist even with the modelling direction shown in Figure 2-2b and c.

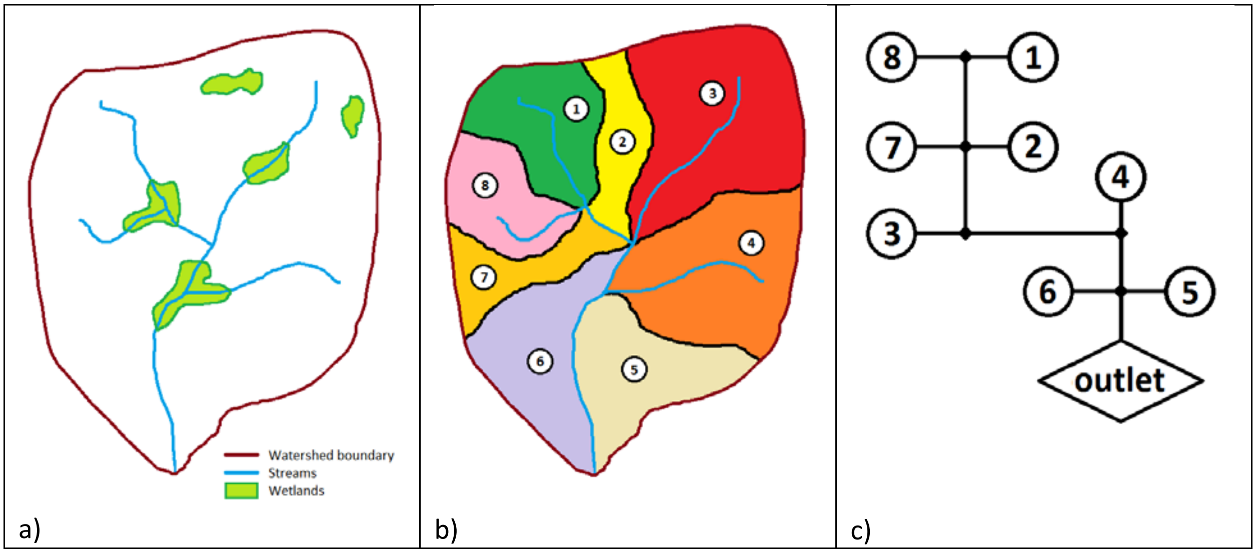


Figure 2-2: An illustration of semi-distributed modelling: a) a conceptual watershed; b) a schematic watershed divided into eight subwatersheds; and c) a topological representation of the schematic watershed divided into eight subwatersheds (see Figure 2-2b).

To create a model that not only accepts distributed inputs, but also distributes the hydrological processes they simulate (i.e., water is allowed to move laterally across landscapes), it is necessary to discretise space into a regular grid (Figure 2-3a) or a flexible mesh (Figure 2-3b). This is an example of distributed modelling in the strong sense and is sometimes referred to as fully distributed.

With this fully distributed model conceptualisation, each grid/mesh cell represents a computational unit, and each cell can be assigned unique characteristics based on attributes such as terrain roughness, vegetation height, surficial soil conditions, land use, etc. Such a distributed model can, for example, simulate runoff in one cell that runs on and infiltrates in cells further downslope, or water infiltrating upslope can recharge the groundwater system and can cause groundwater seepage at a downslope cell causing excess saturation and contributing to overland flow processes. These types of models are able to take explicit account of the runoff-runon phenomenon (e.g., Smith and Hebbert, 1979; Dunne et al., 1991) and groundwater feedback mechanisms (e.g., Dunne and Black, 1970).

For individuals who may be responsible for the review or commissioning of distributed watershed models, it is important to be aware of the processes and interactions that are truly being represented in a distributed manner, and whether the level of distribution is adequate for the modelling objective. It may be helpful to distinguish models referred to in Figure 2-2b as being semi-distributed, since only the forcings are distributed while the land-surface processes are not.

2.3 Other Modelling Concepts

The remaining topics covered in this section relate more broadly to modelling in general, and are not necessarily tied specifically to watershed modelling. However, they are definitely important aspects of watershed modelling and were given considerable attention when SWP models were prepared.

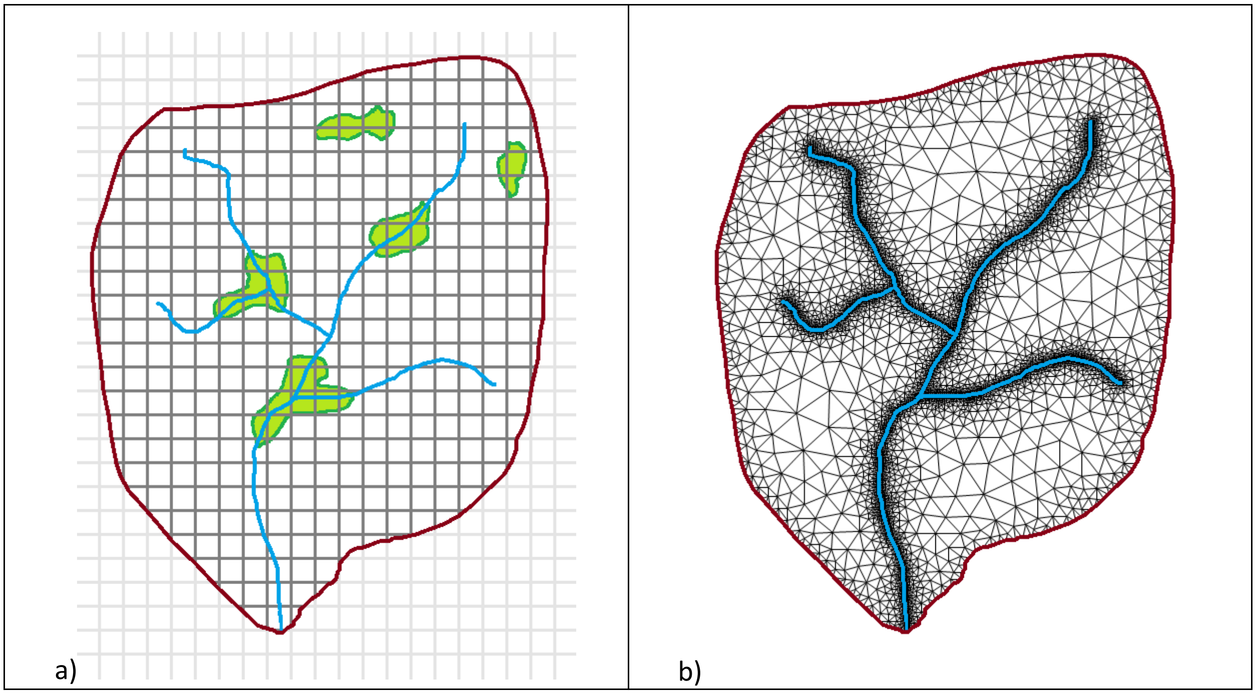


Figure 2-3: An illustration of fully distributed modelling: a) a schematic hypothetical watershed discretised by a superimposed regular grid; and b) a schematic hypothetical watershed discretised using a flexible mesh.

2.3.1 Data

A difficult concept to appreciate in the model-development workflow is the concept of data. In building numerical models, data evolve through a chain of manipulations beginning with raw data, which has been collected in the field, and ending in model results (Figure 2-4). Raw measurement data are cleaned and published as quality-assured data, often by a public agency. Quality-assured data are then processed further to create model-readable input files that will support the conceptualisation, which has been based on expert knowledge of the system being modelled. This process may simply affect the format of the data without changing the information (reversible), or it may require changes that change the information through aggregation and interpolation (irreversible). Each data manipulation step requires choices and provides a source for error, which may have an impact on modelling results.[2] The model code produces outputs that may not be in a format that is easily readable and accessible to the non-modeller. Further processing is then required to translate the output into results/graphs that are interpretable by non-experts and are easily communicated. Any of the steps presented in Figure 2-4 may result in outputs or products that are frequently referred to as 'data'; therefore the reader should be aware that data can come in many different forms.

[2] An often overlooked advantage of numerical modelling is that it provides the best framework for rigorously testing data consistency, and as an outcome, modellers frequently identify data errors when setting up and refining their workflow. Regardless of when in the workflow such errors are detected, they need to be corrected at the appropriate step in the workflow. Once corrected, all subsequent steps need to be appropriately updated. Such correction requires proper documentation and access to relevant knowledge and tools in order to ensure reproducibility in the future.

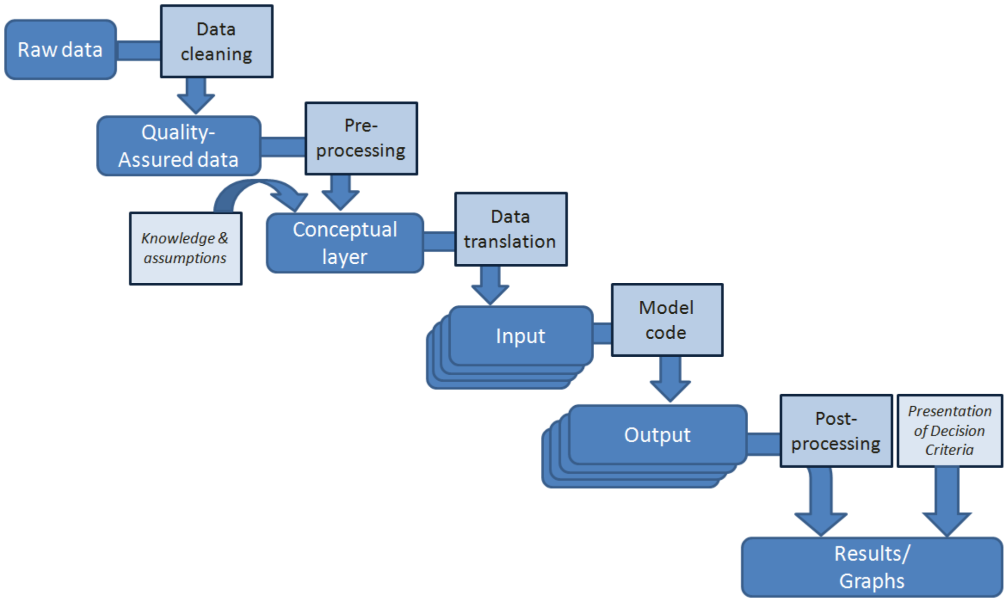


Figure 2-4: A workflow of model elements (dark blue) and processes/steps (light blue) necessary to replicate, test, and/or update results produced through a numerical modelling study.

2.3.2 Model Code

After the physical system has been conceptualised, the modeller must decide on a set of processes, formal rules, and theories that can best represent the system and its behaviour. Since these are built into a set of procedures within a model code, this task generally consists of choosing an appropriate model code. The choice of code must take into account the availability of data, the system conceptualisation, and the modelling objective.

Consideration for the selection of the model code may depend on the future plans that a public agency may have for a proposed model. Jenkinson (2012, p.12, 13) provides an excellent guide on model code selection and suggests the following questions be raised when assessing model-code suitability:

1) Could a simpler or different approach provide better or comparable results?
2) Can the model provide information suitable and sufficient to answer the management objectives and questions?
3) Is the model data appropriate? Can it produce the required output with the available data? Is the overall cost (in time and funds) to acquire necessary data for this modelling exercise sufficiently low?
4) Does the model match the required process representation?
5) Can the model match the dimensional requirements?
6) Can the model operate at the required spatial and temporal resolutions?
7) Can the model operate at the required scale (temporal and spatial)?
8) Can the model readily employ the available data and output data in compliance with the requirements?
9) Does the model have a history of success in similar applications?
10) Does the model have the appropriate complexity for the modelling task?

11) Is there adequate model expertise available to conduct the study?
12) Are there adequate resources (human, financial) to conduct the modelling study within the stated timelines?

2.3.3 Calibration and Validation

As part of the model development phase, model outputs are compared with field-observed phenomena that the model is intended to reproduce. All models contain a number of parameters that can be adjusted/fine-tuned in order for the model to better match observations; this is the process of calibration.

Calibration can be performed manually by the modeller, which generally takes a significant amount of time. Alternatively, modellers can use software that automates certain calibration tasks, which can considerably speed up the calibration process. Even with software, a skilled modeller is still required to oversee and manage this automated calibration process. Once a model is calibrated, it is then common practice to validate the model against observations, preferably using observed data that were not used in the model calibration (Klemes, 1986). Validation essentially builds confidence in the model's ability to predict unobserved phenomena.

2.3.4 Model Assumptions

Every model is a simplification of reality. Modelling expertise comes when modellers understand how simplifications impact and limit their model results. Assumptions are wide ranging, covering everything from how the modeller understands the natural system to how this understanding is translated into mathematical formulation (Crout et al., 2008).

Assumptions involve hypothesising which processes are important versus those that can be greatly simplified or left out entirely. Assumptions also include choices of how processes are simulated, for example, whether to use empirical- or physical-based equations, which temporal and spatial resolution to use, how to numerically solve equations, or how to simplify equations to handle incomplete data. Since all assumptions can impact the model results, the need for clear documentation describing all assumptions cannot be overstated.

For many SWP studies, a peer review committee was employed to corroborate the assumptions made with respect to the modelling objectives and determine whether there was adequate recognition of local knowledge/expertise during the conceptualisation phase of the study.

2.3.5 Initial and Boundary Conditions

In building and running numerical models, the setting of initial and boundary conditions are required. The initial condition specifies the hydrological state of the modelled system before the model is run (e.g., water table is set at a certain elevation, soil is set at a percent saturation, stream stage is set at a specified height, etc.). Boundary conditions are used to represent either input forcing variables to the model (e.g., precipitation) and/or constraints imposed on the model at the edges of the model domain (e.g., no flow boundary, river boundary, lakes, inlets and outlets, etc.).

Technically speaking, models are built from mathematical equations in which initial and boundary conditions are necessary in order to acquire a solution. The experience of the modeller is crucial in determining the appropriate boundary conditions since the boundaries can significantly affect model results (Stephenson and Freeze, 1974). In considering appropriate model boundaries, the modeller may even adjust/limit the scope of the modelling study should adequate data be inaccessible. It should be understood that these conditions can either be data dependent or assumption-based and that any model reporting should include a clear description of how these conditions were derived.

2.3.6 Model Evaluation: Uncertainty and Sensitivity

Since the data used in model development will always be incomplete and models themselves will necessarily be based on simplifying assumptions, model-based predictions will be in error. Uncertainty analysis is a means of quantifying these errors, and it serves to increase confidence and determine the range of applicability in the model results. A rigorous assessment and communication of model uncertainty (typically by providing a confidence range around results) is a sound modelling practice. While the environmental modelling community has reached an overall consensus that all models should adequately address model uncertainty, commonly this is not the case. Beven (2009) conjectures several reasons as to why uncertainty analysis is commonly omitted:

1) uncertainty analysis is not necessary for physically based models;
2) uncertainty analysis is not useful in adding to process understanding;
3) uncertainty (probability) distributions cannot be understood by policy makers and the public;
4) uncertainty analysis cannot be incorporated into the decision-making process;
5) uncertainty analysis is too subjective;
6) uncertainty analysis is too difficult to perform;
7) uncertainty does not really matter in making final decisions.

For these reasons (and perhaps others), accepting uncertainty in model predictions is still not a universally accepted practice. This has led to the situation where many water managers remain ignorant of defensible modelling practices, even to the extent that legislation has been developed contrary to good modelling practices (see Wagner et al., 2010 for U.S. examples). During the SWP program, model uncertainty was generally communicated qualitatively as low, medium, or high. However, this provided little benefit in the development of public policy.

Quite often as part of the model evaluation phase, sensitivity analysis is employed as a means of assessing confidence in model results. With sensitivity analysis, parameters, assumptions, and/or boundary conditions are permuted in order to quantify their effect on model results. Although sensitivity analysis is involved in many uncertainty analysis procedures, it is not an adequate means of assessing model uncertainty in itself, especially with respect to watershed models.

Model evaluation incorporates, in a structured methodology, an evaluation of the processes of model calibration, validation, and uncertainty analysis and is performed after the model has been set-up and run. Objective functions (root-mean squared error, Nash-Sutcliffe, etc.) are statistical tests used to quantify a model’s ability to simulate field data or observations. There are many forms of objective functions, but there exists no universal form and thus the appropriate choice is made by the modeller and depends on the objective of the modelling study.

2.3.7 Empirical- versus Physically Based Models

An issue often raised in hydrological modelling is whether a model is physically (or physics) based.[3] Ultimately, there is no formal definition to the term physically based and thus the term can take on various definitions depending on how a model's processes are handled. For example, a physically based model can be one that:

1) has its numerical formulation of physical process derived from first principles (Yeh et al., 2006) – meaning that model processes are concurrent with scientific theory;
2) is based on physical principles and processes – meaning that the model's formulation and its parameters and variables have some physical interpretation of a system's process-response (Chang, 1988); in principle, the model's parameters should be obtainable through field measurements and the model could become operational with little to no calibration (Grayson and Blöschl, 2000; Neitsch et al., 2011);
3) is scale invariant – meaning that the model's performance will not change regardless of the scale of measurement for variables upon which the model depends[4] (Sposito, 1998);
4) is capable of explicitly simulating a diverse and non-limiting set of watershed/hydrological processes simultaneously, including operational infrastructure (Western and Grayson, 2000; Refsgaard and Storm, 2012);
5) accounts for both mass and energy exchanges and keeps track of variables related to mass and energy over time (Tarboton et al., 2000).[5]

In contrast, empirical models are derived using empirical methods, that is, they are derived from the regression of input-output relationships without an attempt to describe the system processes involved (Grayson and Blöschl, 2000). A classic example of an empirical model widely used in water resources is the rational method that relates rainfall intensity to peak runoff. Empirical models will always contain parameters that don't necessarily have physical meaning. These parameters will always require calibration (i.e., fine tuning) against observed data, and thus empirical models remain largely restricted to the watershed in which they were calibrated.

In practice, however, physically based models tend to include empirical parameters that help to simplify the description of the system dynamics and their governing equations (Julien, 2002), and the distinction between empirical- and physically based models is unclear.

Justification for the use of physically based models comes when attempting to model areas where no calibration data exist, such as ungauged basins. Using a strictly empirical model in an ungauged watershed should be avoided, since there is no guarantee that the results could even be remotely useful when compared to those from a physically based model. That said, it is unlikely that a model

[3] Not to be confused with physical models, which are downscaled physical versions of the system being modelled.
[4] Assuming no increase in heterogeneity with scale.
[5] Commonly referred to as process-based models.

formulation could be produced that would require no calibration, meaning all models are inherently empirical.

2.3.8 Steady-State and Transient Models

The concepts of steady state and transient refer to how a model addresses time. In a steady-state model, the inputs (i.e., precipitation, recharge, etc.) and boundary conditions (stream and lake stage elevation, pumping, etc.) remain constant or steady (i.e., unchanging) through the model run. This is a useful modelling approach when attempting to assess the average state of an environmental system. In a transient model, the input variables and/or boundary conditions can change at any time step, and the model's state will transform in response to these changes. This model will progress through time, more closely reflecting reality. This form of modelling is useful when attempting to determine the progress of a dynamic phenomenon, for example, a flood wave or groundwater contamination.

3 A CYCLIC APPROACH TO MODELLING

3.1 OVERVIEW

Adaptive policy making is becoming integral to water management as the understanding of hydrological systems continues to be reshaped in response to changing environmental conditions, evolving sociocultural perspectives, and the emergence of new technologies. Within Ontario's water sector, numerical modelling, which will increasingly play an important supportive role in adaptive policy making, has become a prescribed tool for water management as mandated by the Clean Water Act, 2006 (Ontario Legislative Assembly, 2006). However, numerical modelling has proven to be a technical and organisational challenge for public sector agencies. Projects commissioned under the source water protection (SWP) program have in many cases run over budget and/or missed set deadlines. After the significant investment that has gone into these projects, there is concern that these numerical models will be shelved after their one-time use, thus preventing others from reaping all the insights and benefits that these models could potentially provide.

Drawing from experiences with the SWP program, this guide recognises that numerical model development should be considered as a cyclic or iterative process, requiring periodic updates to the understanding of the hydrological flow system and refinement of models.[6] For large-scale watershed management, in particular, it is recommended that agencies take into consideration the longer term usability of numerical models, as well as the longer term benefit that can be derived from isolated model components (e.g., the assembled data, interpreted surfaces, material properties, etc.).

This perspective of an iterative, learning-oriented process rather than a linear, outcome-oriented process redefines the objective of modelling from providing the 'truth' to providing a more formalised summary of the current limited knowledge of the system. This has an influence on many aspects of numerical model development, including:

- the design and selection of software codes;
- the management of both data and knowledge within public sector and consulting organisations;
- the set-up and costs of the modelling project;
- the need to address intellectual property rights in a more robust manner; and
- the interchange of knowledge with external partners.

The iterative approach has some key implications on model management. It will:

- eliminate the perception that revisiting a model conceptualisation after a model has failed to perform as expected is an overall modelling failure – rather this will be viewed as part of the learning process that leads to new insights and opportunities;

[6] This cyclic approach deviates from a linear list of modelling steps, currently in use by European water managers who are implementing the Water Framework Directive (e.g., Refsgaard and Henriksen, 2004; Jakeman et al., 2006; Vanrolleghem, 2010). All of these authors point out that modellers frequently have to revisit and repeat earlier modelling steps, however, they continue to maintain a linear perspective on numerical modelling.

- require access to expert knowledge on a repeated basis, such that model managers would seek to establish improved longer term collaborative relationships with modelling consultants;
- require investment in a long-term centralised data infrastructure, which will greatly increase data accessibility and reduce costs related to future modelling projects;
- require investment in other centralised knowledge management activities, such as the implementation of cyber infrastructure for ready access to models, enhancement of model-related responsibilities for agency staff, and the standardisation of model custodianship and archiving procedures; and
- reduce automation costs through efficient coding/scripts/software for specific technical modelling steps, thus allowing for efficient rerunning of models which will lead to improved system understanding and scientific defensibility of model-based decisions.

3.2 Three Embedded Cycles/Iterations

Figure 3-1 provides a high-level framework for conceptualising how numerical models can be iteratively used in the larger context of water resources management and introduces three interdependent cycles: the policy cycle; the conceptual learning cycle; and the technical modelling cycle. The following sections elaborate on the three cycles, and how they link with each other.

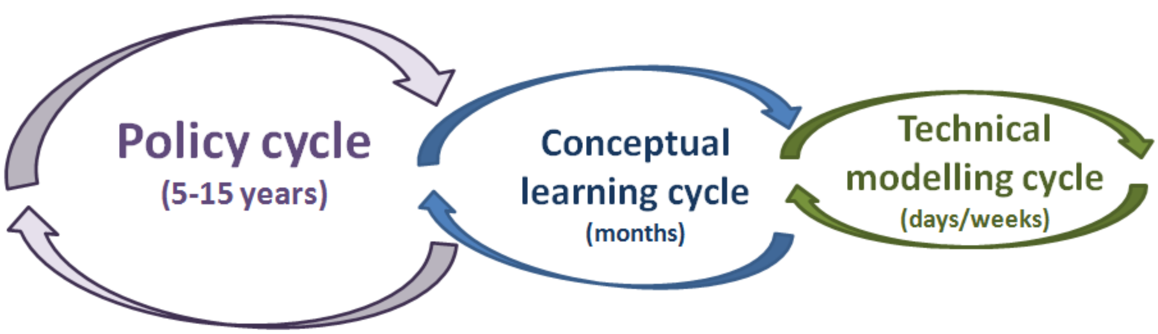


Figure 3-1: Numerical modelling in the context of three interdependent cycles: policy, conceptual learning, and technical modelling.

3.2.1 The Policy Cycle

Typically, the policy cycle, where water management policies are deliberated and set, is a core responsibility of public sector agencies. If existing policies, developed without numerical model support, are not proving effective in addressing water resources concerns, then it is at this stage where the need for numerical modelling can be first identified. Numerical models would only be used at this stage of management if they were already available from a previous study. Proposed policies can be evaluated considering a model-based assessment, implemented, and the outcomes monitored in preparation for the next time the policy would be reviewed. Modelling may also be used at this stage to design monitoring programs to help in the assessment of policy effectiveness.

Although it may seem external to numerical modelling, the formal consideration of the policy cycle places an emphasis on the importance of using numerical models as tools to help shape water resources management policy. Agencies across the globe have turned to adaptive management as a planned and systematic strategy for continually improving environmental practices and for assessing and improving water resources–related policies. Adaptive management provides a flexible framework to monitor responses to policy enactment, evaluate and learn from the monitored observations, and then identify and implement new policies, or modify existing ones, during one program cycle (Canadian Environmental Assessment Agency, 2010).

The driver for initiating a policy cycle is typically a water resources issue (e.g., flooding, poor water quality, etc.) that society demands be addressed. Through the policy cycle, society expects the issue to be effectively addressed in a fact-based and cost-effective manner. Typical steps of the water resources management policy cycle are shown in Figure 3-2 and include:

1) Formulate clear policy goals – this step involves the evaluation of water resources within the area of interest and the development of clear policy goals to change the way the resource is managed (e.g., reduce nitrogen loading in water courses). In addition to establishing these goals, this step would also justify the need to make use of a numerical model to assist in setting effective policies.
2) Prepare scientific assessment – this step involves technical work required for the construction of a numerical model and incorporates both the conceptual learning and the technical modelling cycles.
3) Design policies – various alternative policies can be run through the model to evaluate their predicted effectiveness in meeting the set goals. While the model can help in quantifying risks and trade-offs amongst conflicting policies, it is an explicit societal decision to review the effectiveness of each evaluated policy in meeting the goals and to make a final implementation decision.
4) Implement policies – once the modelling work is complete and the selected policies have been agreed upon, then they are implemented on the landscape to better manage water resources.
5) Monitor responses – with the onset of policy implementation, monitoring of the responses of water resources to the policies must be undertaken in order to assemble the observation data required to evaluate the effectiveness of the implemented policies. Note that the design of the monitoring network could also be established and optimised with the assistance of the numerical model.
6) Evaluate policies – as new information is collected, the data must be assessed on a regular basis to look for indications of how the implemented policies have influenced or changed water resources.

Deliverables from the policy cycle include: i) potential policy options that could be implemented to address an issue; ii) an evaluation of those options, in the context of this document that would mean evaluation through the use of numerical modelling; and, finally, iii) an implementation and monitoring plan for the preferred option(s) selected as best to help in addressing the water resources issue.

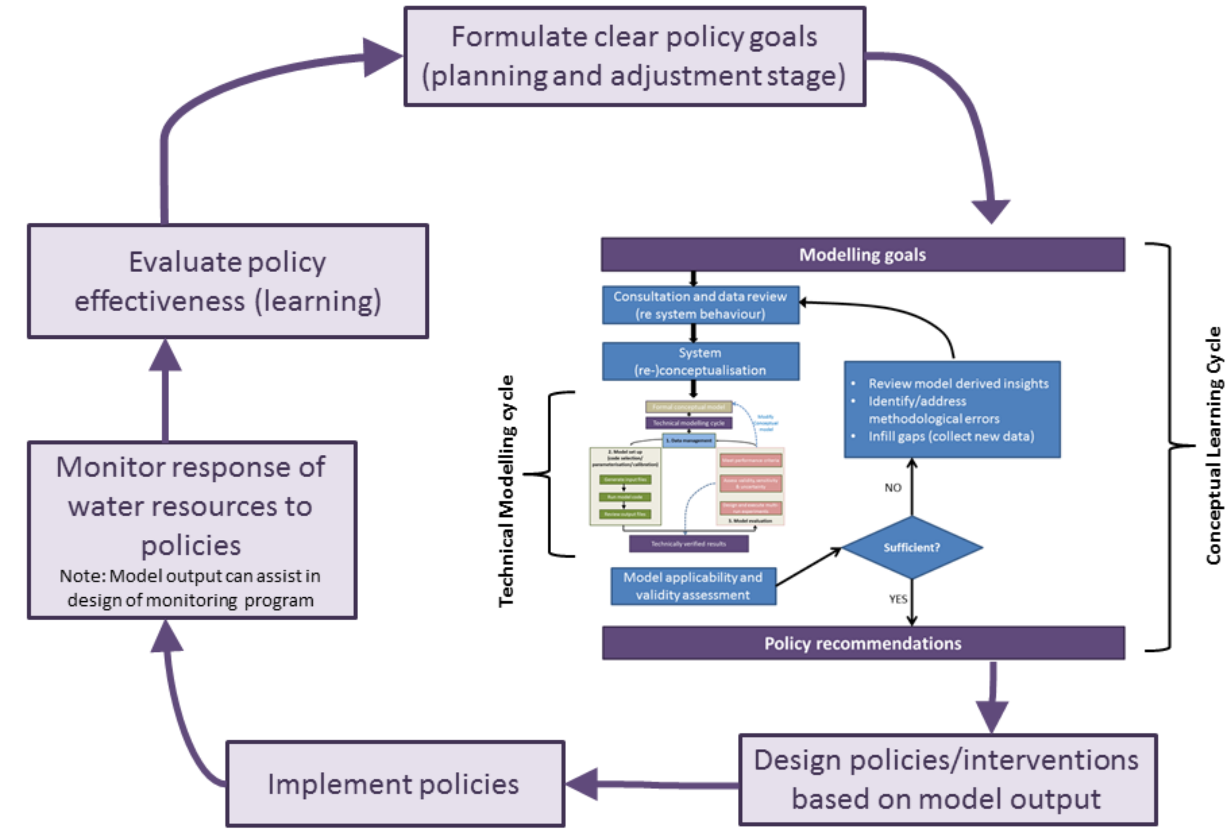


Figure 3-2: The main steps of the water resources management policy cycle.

Overseeing the policy cycle requires a wide ranging skill set including: i) an understanding of the agency's legal and governance systems; ii) practical planning knowledge of how to design various policy options and eventually implement the preferred option(s); iii) technical knowledge to direct modellers in the design and assessment of various policy alternatives using the numerical model; and iv) communication skills to effectively work with the many stakeholders and parties who provide input to water resources management. The policy cycle would typically be led by planning staff from a public sector agency with wide ranging technical input from other stakeholders.

3.2.2 The Conceptual Learning Cycle

At the conceptual learning cycle, agencies are preparing for numerical modelling and the focus is on system conceptualisation. Ideally, this cycle involves the collaboration of a wide variety of contributors, ranging from local residents to agency staff (both technical and planning) to academics and consultants. They will have: i) relevant hydrological knowledge of the flow system to be modelled; and/or ii) targeted questions or policy scenarios that the model is ultimately going to help address. With this broad input, the goal of this phase is to compile the knowledge of various subdisciplines into a coherent and science-based conceptualisation of the system. Using a groundwater model as an example, the conceptualisation might involve, amongst other elements, determining how many layers are needed to adequately capture the subsurface variability in aquifers and aquitards.

The developed conceptual model is passed to the modellers who then become responsible for translating the conceptual model into numerical model input files, and for the subsequent technical model implementation. As such, the conceptual learning cycle is very much interwoven into the technical modelling cycle and for many modelling projects it may indeed be difficult to separate it out as a distinct component. However, the cycle is isolated or removed from the technical modelling cycle simply because it typically involves a wider range of professionals that provide input, all of whom should agree to any conceptualisation changes needed to improve the modelling process.

As numerical model output and results are reviewed, it is recommended that changes to the system conceptualisation happen within the conceptual learning cycle and are subsequently run back through the technical modelling cycle. From experience in practical modelling projects, including those undertaken for Ontario's SWP work, it is common for the technical modellers to make adjustments to the conceptualisation as they run and rerun the model to achieve desirable results. By formalising the conceptual learning cycle, these types of ad-hoc conceptual model adjustments, unless they are very minor in nature, are discouraged. The preference being that any significant conceptualisation changes that benefit the technical modelling work should come back to a wider group for approval prior to their implementation. To develop this type of interaction, it could perhaps be specified within the RFP that monthly meetings be scheduled for the duration of the project (and perhaps only be used as necessary) so that the technical modelling process is not hindered by consultation requirements.

Figure 3-3 shows the main steps involved in the conceptualisation cycle:

1) consultation and data review – initial widespread consultation regarding the flow system behaviour;
2) system conceptualisation – review of available data/knowledge to develop a conceptualisation of the system to be modelled;
3) model applicability and validity assessment (if needed) – input into assessment of technical model outputs to ensure model applicability and validity;
4) reconsider conceptualisation (if required)
    a) evaluate insights from technical modelling work;
    b) identify and address methodological errors/oversights; and/or
    c) review data and, if needed, collect new data to infill gaps in system understanding.

Deliverables of the conceptual learning cycle are restricted to the conceptualisation (or reconceptualisation) of the system to be modelled. This could be summarised in minutes of consultation meetings, and sometimes a separate conceptual model report is prepared that can be used by the technical modellers as they create the input files for the model.

The conceptualisation cycle requires a broad range of knowledge regarding the system to be modelled, ranging from highly technical scientific insights to more generalised local knowledge. This type of widespread consultation provides an ideal opportunity to capture a qualitative description of the system (e.g., "the stream is always dry at my property in July") that can be used by the technical modelling team as a constraint when building the technical model. The conceptualisation process would tend to be best

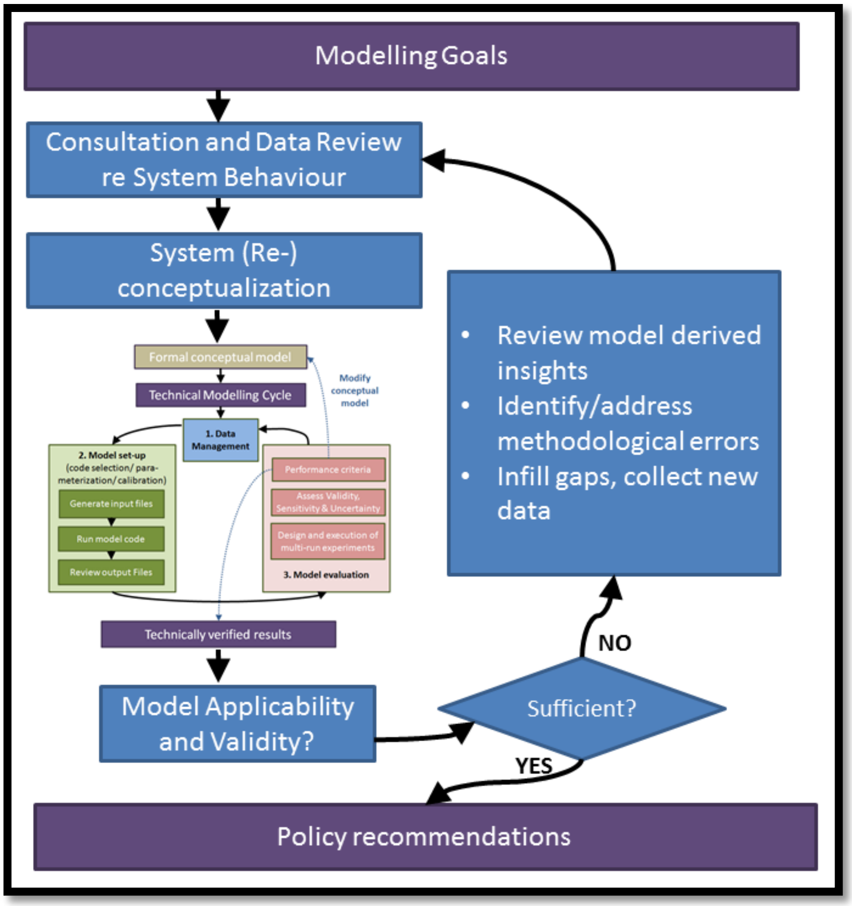


Figure 3-3: The main steps involved in the conceptual learning cycle.

led by agency technical staff, with technical modelling experts providing higher level modelling input. Policy support would be provided by less technical staff (e.g., from planning, environmental, etc.) who are involved in setting water management policies.

3.2.3 The Technical Modelling Cycle

Within the technical modelling cycle, modellers translate the conceptualisation of a system into a numerical model. Once the model is built and validated as being applicable to assist in understanding the hydrological system under investigation, various scenarios (including policy related) can then be evaluated. With an eye to the agency's modelling objectives and goals, to successfully execute the technical modelling work, practitioners must have: i) an understanding of data formatting, processing, and storage; ii) a sound understanding of the system conceptualisation; and iii) an in-depth knowledge of technical aspects of the modelling process. Individuals involved in the technical cycle are typically consultants.

Figure 3-4 illustrates the main steps or the scientific workflow within the technical modelling cycle. The three main steps include:

1) data management – design and establish a database for storing and accessing data;

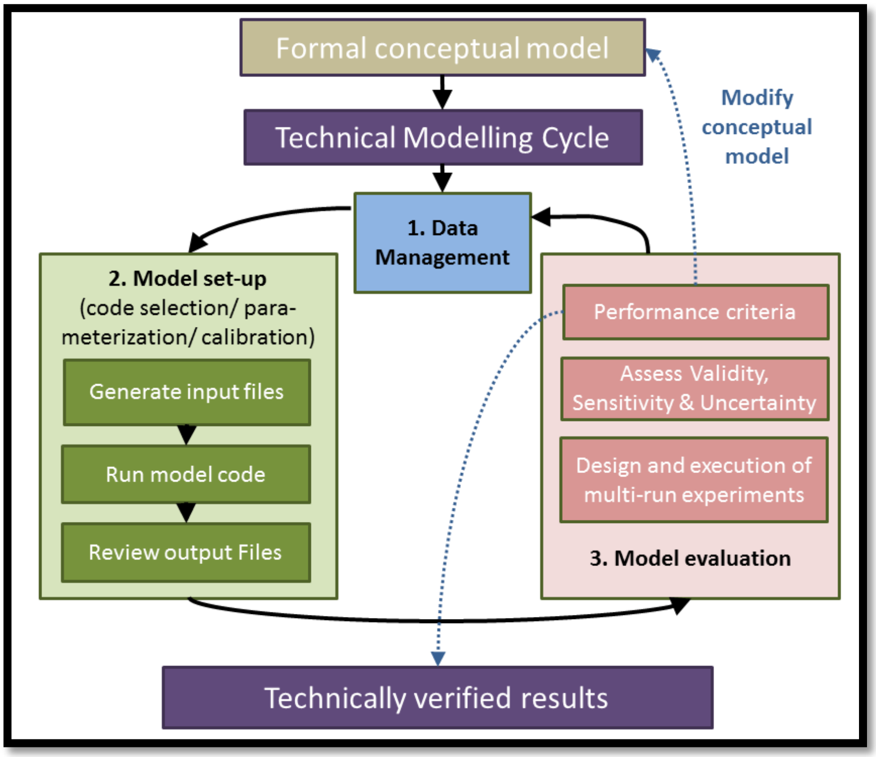


Figure 3-4: The main steps of the scientific workflow within the technical modelling cycle.

2) model set-up (code selection/parameterisation/calibration) – model is built to reflect the site (e.g., watershed, regional area, proposed development site, etc.) as best as possible, and subsequently run many times, continually working to calibrate model parameters and to verify the model applicability. In running the model, workflow substeps may include:
    - generate input files;
    - run the model code;
    - review output files, adjust model components or parameters as necessary and rerun;
3) model evaluation – includes systematic procedures for verifying the technical modelling work and for assessing model uncertainty.

Deliverables of the technical modelling cycle are:

- the collected data and organised database with relevant data;
- a working numerical model;
- a final model report documenting:
    - the conceptualisation of the model;
    - the processes, procedures, and assumptions made in developing the model;
    - the model results;
    - the modelling workflow, specifically highlighting how model results were created and could be recreated, if needed;

- o the model evaluation, including elements such as model validation, meeting performance criteria, uncertainty analysis, sensitivity analysis; and
- o the model's future applicability outside of the scope of the current project.

3.3 The Three Cycles within a Drinking Water Source Protection Context

Ontario's SWP program has presented important opportunities to improve water management and has provided lessons that remain at the cutting edge of attempts to strengthen the use of modelling tools by water management agencies. The provincial Clean Water Act, 2006 (Ontario Legislative Assembly, 2006), outlines an adaptive management approach, which encapsulates all three cycles. The overall SWP program was organised along the steps of the policy cycle (outlined above):

- Formulate clear policy goals – following on the Walkerton tragedy, a water resources management problem (lack of source water protection) was clearly articulated in Justice Dennis O'Connor's *Report of the Walkerton Inquiry* (O'Connor, 2002a, b). With a policy goal of improving source water protection, the Province issued a set of Technical Rules to guide agencies in preparing *Terms of Reference* documents to address the problem. The use of numerical modelling was explicitly introduced as a means of addressing the water resources management issue.
- Prepare scientific assessment – as part of SWP characterisation reports, and sequential tiered follow-up technical investigations, agencies were required to undertake technical work to summarise existing water resources data and knowledge, and to prepare scientific water resources assessment reports (making use of numerical models if warranted) that identified threats to both water quantity and quality.
- Design policies – SWP committees collaboratively developed policies to address the documented threats.
- Implement policies – to address each threat, the committees assessed and selected the best policy and identified the agency responsible for the policy implementation and enforcement.
- Monitor responses – ongoing and future water resources monitoring to assess the effectiveness of policies are anticipated to become an important element of the source protection plan.
- Evaluate policies – into the future, the SWP committees will evaluate whether enacted policies have been effective in addressing drinking water threats. Results of the evaluation will be considered in future when revisiting the policy cycle.

The scientific assessment component of the SWP policy cycle made use of numerical models to better understand and assess the watershed flow systems associated with:

- groundwater-based municipal drinking water systems;
- surface water intakes; and
- wells where groundwater is under the influence of surface water.

The SWP reports identified drinking water quality threats that could be tied to these water supplies and, in a parallel work stream, also identified water quantity threats using a three-tiered approach. The first tier used a simple water budget approach to determine water stress or scarcity within watersheds that had municipal drinking water intakes (wells or surface water). Applying the precautionary principle, watersheds meeting a certain current and/or future stress threshold were flagged for additional tier 2 investigation. Using numerical models (with no dynamic coupling), the tier 2 work was focussed on assessing water availability to wells and/or surface water intakes. Water supplies that were modelled as being potentially unable to meet current or future long-term water supply needs were then subjected to a more detailed tier 3 integrated or coupled modelling approach. This three-tier water budget process limited the use of very complex and integrated models to only specific parts of the province, thereby optimising the use of financial and technical resources.

The conceptual learning cycle was generally led by a consultant, in one of a variety of partnership arrangements with the local SWP committees and the staff from affected municipalities and conservation authorities.

The technical modelling phase followed and was undertaken by the same consultant. This consultant introduced procedures for managing/converting data, calibrating models, experimental design, output evaluation, and the generation of results. Reproducible routines were generated through the modelling process, and included the creation of model input from available data and the generation of output by running the model code multiple times. For surface water assessments, backward tracking of particles was determined under varying wind scenarios and the multiple backward tracking results were superimposed to ultimately generate files that best described the intake protection zones (IPZs). For groundwater assessments, backward particle tracking routines were readily available to delineate wellhead protection areas (WHPAs). A variety of modelling software codes and approaches were used across the province. Unfortunately, there was little standardisation with respect to contracting, deliverables (including the models themselves), and reporting. Although the Clean Water Act, 2006, (Ontario Legislative Assembly, 2006) requires public sector agencies (municipalities or conservation authorities) to maintain the numerical models for a set period of time into the future, there was little direction provided, no recognition of the challenges posed, and no long-term planning established to work with and improve the models following the SWP program. The intention of this guide is to help fill this void.

A key component of the modelling work was a peer-review process. A peer-review committee, consisting of local experts, academics, and other consultants, was put in place to review technical modelling work. The peer-review committee raised conceptual and technical questions, suggested technical improvements, and also highlighted knowledge gaps to be addressed. For the simpler qualitative threat assessment modelling, model documentation was reviewed by contracted external reviewers. The SWP committee and public stakeholders provided a local perspective and commented on high-level issues related to model development.

4 GOVERNANCE AND LEGAL CONSIDERATIONS

With respect to managing numerical models, a general state of unpreparedness currently exists at public sector agencies following the implementation of Ontario's source water protection (SWP) program. So many numerical watershed-scale models were commissioned in Ontario over such a short time span and it is apparent that there is an imperative need for the long-term management of these numerical models. There is also a need for policies to assist in the longer term effective use of the models.

Given Ontario's situation, one of the first governance-related issues to be considered when setting out on a numerical modelling pathway is for public sector agencies to recognise the potential long-term usability and benefits that will result from a model, and to consider the following points prior to commissioning a new model:

- Are there already pre-existing models that can be used to address the problem at hand?
- Should other agencies be invited to become partners in a modelling study?
- Can the model study be broadly scoped such that other levels of government can provide funding to support the model study?

The following discussion touches upon some governance and the intertwined legal aspects related to commissioning new models, and managing or making use of existing numerical modelling. Water resources decision-makers at public sector agencies are now in a position to capitalise on earlier modelling investments, and to move forward with integrating models into their day to day work. With this comes a need for direction as to how best address a number of governance issues, which are now emerging across the province. Numerical models reflect a significant capital investment and, like other assets, should be considered a form of infrastructure in need of long-term maintenance. Public sector agencies can incorporate the ideas presented below into their ongoing practices to manage their models as tools that regularly inform decision-making.

Topics and related questions that come to the fore in terms of model governance include:

- Ownership – Who owns the models?
- Custodianship – Who will ensure the model has been delivered in its entirety and manage it in the long term?
- Managing model updates – How will changes to the model be addressed and under whose authority?
- Accessibility and sharing – Which organisations (either private or public) have the right to make use of the models?
- Technical capacity and expertise of staff – Where does the capacity reside to effectively make use of the models?

These issues are addressed in this section.

4.1 REQUEST FOR PROPOSAL AND LEGAL CONTRACT DOCUMENTS

As stated earlier (Section 1.8), the most successful modelling projects are those in which staff from public sector agencies and modelling consulting firms are working in partnership, having mutual respect for the skills and input that each party brings to the project. In order to foster such a collegial atmosphere and to prevent misunderstandings, which sometimes only emerge part way through a study, it is important that both the Request for Proposal (RFP) document and the legal contract documents clearly articulate the expectations and the deliverables from the modelling study. Problems tend to arise when consultants bid on a project without having a clear understanding of the client's expectations. This can result in insufficient funds available to deliver the client's expectations.

In addition to clearly define the scope of the project from a technical perspective, the RFP should also clearly convey the agency's intentions, in particular, with respect to the longer term use of the model.

4.1.1 Recommendations for Request for Proposal (RFP) Documents

A comprehensive and detailed RFP can be a great asset and reference throughout the modelling process. Appendix 3 provides examples of clauses that can be incorporated into these RFPs. The following key directives are addressed in detail within the appendix:

- convey your agency's long- and short-term intentions for the use of the model;
- convey your agency's need for proper data management;
- directly address intellectual property rights;
- directly address eventual model ownership;
- address the issue of modified model codes;
- address the issue of potentially proprietary scripts and other software products that enable the creation of final modelling results;
- directly address the notion of file transfer;
- specify file transfer to agency's computers;
- include knowledge transfer plan; and
- consider the issue of longer term file back-ups.

4.1.2 Recommendations for Legal Contract Documents

It is a good management practice to incorporate key clauses into legal agreements to ensure understanding by both parties as to the expected deliverables or outcomes from the project. Some of the wording that is drafted for the RFP can be adapted for incorporation into a legal agreement.

Appendix 3 provides examples of legal clauses that can be incorporated into an agreement to address the following modelling related topics:

- ownership of model and associated files;
- defining intellectual property;
- transfer of intellectual property;

'CASCADING' LEGAL AGREEMENTS

From the provincial perspective, a significant issue that arose during the source water protection (SWP) program was the issue of what is coined here as 'cascading' agreements. The issue arose owing to the fact that legal clauses in a Provincial – Local Agency agreement were not carried forward into subsequent Local Agency – Consultant agreements. After entering into a legal agreement with the Province, local agencies would receive provincial funding and would then be responsible for ensuring that numerical modelling projects were carried out to the Province's expectations. Although the Province may have incorporated specific 'ownership' or 'intellectual property' clauses into their agreement with the agency who received funding, commonly these clauses were not carried forward into subsequent agreements. As a direct result of these clauses not being included in the Local Agency – Consultant agreements, consultants prepared proposal documents and undertook their modelling work unaware that the Province was seeking to take ownership of the intellectual property resulting from their work.

The issue is clearly one of poor communication and could readily be resolved through one of several ways, two of which are:

1) within the Province – Local Agency agreement, the Province clearly specify one section (perhaps entitled 'Cascading Clauses') under which any clause in this agreement would be mandated for carry forward into any subsequent agreements entered into under the funding arrangement; or
2) through a program website and/or various bidders meetings hosted by provincial staff, the Province could inform the broader consulting community of the Provincial intent to retain intellectual property rights for any numerical modelling undertaken under the broad scope of the program.

- addressing consultant intellectual property; and
- addressing multiple agencies funding a modelling study.

The clauses found in Appendix 3 are adapted from previously reviewed contract documents. The sections below also provide some examples of ownership-related legal clauses that have been extracted from reviewed legal documents. It is strongly recommended that any agency have their legal counsel review and approve of legal clauses found within this guide prior to their use.

It is highly recommended that both the Request for Proposal document and the successful consultant proposal be appended to any legal agreement prepared between the consultant and the client agency.

4.2 Ownership/Intellectual Property Rights

The issue of ownership is most important where the intention is to make use of the model into the future. For situations where a model is constructed for a one-time use analysis, ownership is typically not considered to be a priority.

The importance of identifying the owner of any numerical model (whether it is a public sector agency or consulting firm) is that the model owner is deemed responsible for two important post-modelling decisions:

- how the model can be used in the future (i.e., for what projects); and
- who (consultants, other agencies, public, etc.) is able to use the model.

NUMERICAL MODEL OWNERSHIP/INTELLECTUAL PROPERTY RIGHTS

Science-based environmental modelling is an arena where scientific principles are weighed against entrepreneurial interests. On the one hand, scientific principles state that science-based products and procedures should be widely distributed for thorough review and that unrestricted access to models and related software tools would help to improve model reproducibility and validate the results. On the other hand, within the private sector, it is generally accepted that models and computer code developed for commercial endeavours is to be privately held and maintained as a competitive advantage for future gain.

Although numerical modelling makes use of commercial software code, unmodified code is not the focus in this guide. Rather, it is the building of model elements (e.g., hydrostratigraphic layer construction, hydraulic property assignments, etc.) and the combining of all of these elements to create the numerical model that constitutes the intellectual property referred to in this document.

Intellectual property or intellectual assets include inventions, new technologies, new brands, original software, novel designs, unique processes, and more. In Canada, these assets can be protected through the use of patents, industrial designs, trademarks, copyright, or trade secrets. The Canada Business Network (http://canadabusiness.ca/government/copyright-and-intellectual-property/what-is-intellectual-property/) defines intellectual property as follows:

> *Intellectual property refers to the legal rights to ideas, inventions and creations in the industrial, scientific, literary and artistic fields. It also covers symbols, names, images, designs and models used in business.*

In Ontario, the issue of model ownership does not appear to have been a concern in the past owing to the fact that one numerical model has rarely been used for multiple studies. So the issue is a fairly recent one. Upon review of several contract documents that have been used for numerical modelling studies, there is a wide range in approaches to the handling of numerical modelling ownership. In general, when a consultant prepares a contract, the ownership clauses point to the consultants (or jointly, the consultant and the client) as the owner of the model/intellectual property rights. In cases where the public sector agency prepares the contract, the agency is identified as the model owner or ownership is not specified.

To avoid misunderstandings, it is recommended that when embarking on numerical modelling studies, all parties involved must be made aware of the possibility of a model being used for more than one study. Therefore ownership of the model/intellectual property rights must be openly discussed and agreed upon at the Request for Proposal and contract stage of the study.

4.2.1 Modified Model Codes

Sometimes, when presented with a unique modelling challenge, consultants will modify existing modelling software code in order to fulfill project expectations. Many model codes used in practice are available in open-source format, meaning that the code is accessible to model users and thus can be readily modified to meet specific needs. In contrast, other codes (proprietary) are closed-source or off-the-shelf, meaning that the codes cannot be modified. The utility of these closed-source models is therefore restricted to the processes for which the model code was designed. For most typical modelling applications, proprietary codes will be found to be well suited to provide a solution, and it is only in rare cases that code modification may be required and therefore it is generally discouraged. The United States Geological Survey provides a reasonable approach for cases where code has been modified (see inset box below).

CODE MODIFICATION: LEGAL REQUIREMENTS

When code is modified, the original model code developers often require that modifications be disclosed. Organisations like the United States Geological Survey (USGS) make modelling software freely available for "use in the public interest and in the advancement of science," as well, they provide support tools for setting up models and visualising results. Included with every USGS download is their Software User Rights Notice (http://water.usgs.gov/software/CAP/code/1.0/UserRightsNotice.html), which states:

> *Software and related material (data and (or) documentation), contained in or furnished in connection with a software distribution, are made available by the U.S. Geological Survey (USGS) to be used in the public interest and in the advancement of science. You may, without any fee or cost, use, copy, modify, or distribute this software, and any derivative works thereof, and its supporting documentation, subject to the following restrictions and understandings.*
>
> *If you distribute copies or modifications of the software and related material, make sure the recipients receive a copy of this notice and receive or can get a copy of the original distribution. If the software and (or) related material are modified and distributed, it must be made clear that the recipients do not have the original and they must be informed of the extent of the modifications. For example, modified files must include a prominent notice stating the modifications made, the author of the modifications, and the date the modifications were made. This restriction is necessary to guard against problems introduced in the software by others, reflecting negatively on the reputation of the USGS.*
>
> *The software is public property and you therefore have the right to the source code, if desired.*
>
> *You may charge fees for distribution, warranties, and services provided in connection with the software or derivative works thereof. The name USGS can be used in any advertising or publicity to endorse or promote any products or commercial entity using this software if specific written permission is obtained from the USGS.*
>
> *The user agrees to appropriately acknowledge the authors and the USGS in publications that result from the use of this software or in products that include this software in whole or in part.*
>
> *Because the software and related material are free (other than nominal materials and handling fees) and provided "as is," the authors, the USGS, and the United States Government have made no warranty, express or implied, as to accuracy or completeness and are not obligated to provide the user with any support, consulting, training or assistance of any kind with regard to the use, operation, and performance of this software nor to provide the user with any updates, revisions, new versions or "bug fixes".*
>
> *The user assumes all risk for any damages whatsoever resulting from loss of use, data, or profits arising in connection with the access, use, quality, or performance of this software.*

4.2.2 Existing Modelling Studies

In reviewing several legal contract documents that have been recently prepared by either public sector agencies or consultants, generally one of the seven approaches outlined below has been taken to address model ownership/intellectual property rights:

1) There is no mention of model ownership nor is there any specified requirement for the model or any files to be transferred. Documentation with respect to intellectual property/model ownership is simply not included. In some cases, municipalities or conservation authorities commissioned the modelling studies prior to the onset of the SWP program or without Provincial financial support or technical oversight. In such cases, particularly where future use of

the model is anticipated to be in the interest of the public sector agency, it is recommended that the consultant be contacted and an agreement reached as to the transfer of the intellectual property rights (i.e., ownership/rights to use the model) to the public sector agency. It should be noted that in cases where the modelling study is older (approximately five years or more since completion) and where the model files have not been transferred to the public sector agency, there could be a significant cost incurred by the consultant to find and recover the older files and to ensure that they reflect the results conveyed in the reporting. The consultant would obviously be justified in passing labour costs associated with file retrieval onto the requesting agency.

2) The agreement (prepared by the Province, as the client) explicitly expresses that the client agency is not interested in retaining the use of the model for future work and that ownership of the model does not have to be transferred. For SWP program studies in which the Ontario Ministry of the Environment and Climate Change (MOECC) was the agency leading a modelling study, the intellectual property rights have been declined by the Province. This includes those studies undertaken under a Transfer Payment Agreement (TPA). In these cases, the ownership of the model likely resides with the consulting firm that was retained to build the model. However, it could also be argued, that in declining to accept the ownership of the model, the MOECC was, by default, transferring ownership to the local municipal government or conservation authority leading the modelling study.

    ***"Agency Name** is not the owner of any intellectual property generated as a result of the Agreement."*

   If public sector agencies want a model to be available for use in the future, it is again recommended that the public sector agencies involved contact the consultant to inquire whether they would agree to officially transfer the model ownership to the public sector agency.

3) The agreement (prepared by the Province [client]), through generalised wording, requires delivery of files to the public sector agency, however, there is no mention of model files specifically, nor is there mention of the ownership of the model.

    *"Upon termination of this Agreement, all documentation relating to the Project shall be delivered to **Agency Name** including, but not limited to, all work product, drawings, paper and electronic files."*

4) The agreement (prepared by the Province [client]) does not specifically mention models or modelling files or their transfer, however, it does legally require that ownership of all intellectual property (which would include any models created through the project) to be transferred to the public sector agency. In the cases reviewed, consideration of the consultant's pre-existing intellectual property (e.g., any software or model coding scripts generated prior to the project) used in the model is given due consideration (e.g., it must be made available to the client at a cost to be determined). For SWP studies in which the Ontario Ministry of Natural Resources was the agency leading the study, the intellectual property rights/ownership of the model have been retained by the Province. This applies both to modelling studies that were commissioned either with a Memoranda of Agreement (MOA) or with a Consulting Services

Agreement (CSA). In these cases any municipal government or conservation authority involved with the modelling study would likely have full access to the use of the model for future work. A letter outlining the intent to use the model might be required by MNR staff so they can keep track of ongoing model use.

*“**Agency Name** shall be the sole owner of any Newly Created Intellectual Property. The Supplier irrevocably assigns to and in favour of **Agency Name** and **Agency Name** accepts every right, title, and interest in and to all Newly Created Intellectual Property in the Deliverables, immediately following the creation thereof, for all time and irrevocably waives in favour of **Agency Name** all rights of integrity and other moral rights to all Newly Created Intellectual Property in the Deliverables, immediately following the creation thereof, for all time. To the extent that any of the Deliverables include, in whole or in part, the Supplier’s Intellectual Property, the Supplier grants to **Agency Name** a licence to use that Supplier Intellectual Property in the manner contemplated in this Article, the total consideration for which shall be payment of the Rates to the Supplier by **Agency Name**. Drawings and documents, or copies thereof, required for the Project shall be provided to **Agency Name** on a monthly basis or more frequently as required by **Agency Name** staff.”*

*“Documents prepared by the Consultant may be used by **Agency Name**. **Agency Name** shall have the sole and exclusive title to the drawings, reports, specifications, and any other documentation prepared in connection with the Project. The Consultant shall be entitled to retain a copy of all documents and drawings produced for the Project but shall not disclose or release any drawings, documents, specifications, and any other documentation prepared in connection with the Project, or copies thereof, to any person or organisation without the prior written consent of **Agency Name** at any time before, during, or after the completion of the Project.”*

5) The agreement (prepared by the consultant), through unclear language, transfers the rights to the project “deliverables” to the public sector agency (client) or to be held jointly by the “study partners” (where study partners is interpreted to be the client and the consultant).

   *“The rights to all deliverables are to be assigned to the **Client**. All deliverables and information to be provided under the terms and conditions of this Project shall be the absolute property of the **study partners**. The **study partners** shall have sole ownership of copyright and other intellectual property rights in all these deliverables.”*

6) The agreement (prepared by the consultant) explicitly expresses that the copyright is to be retained by the consultant with the public sector agency (client) granted use of the documents. No specific mention of electronic model files is provided, however, the consultant could make a link between “documents on electronic media” and model files.

   *“All documents, including documents on electronic media, prepared by the **Consultant** in connection with the Project are instruments of service for the execution of the project. The **Consultant** retains the property and copyright in these documents, whether the project is executed or not. The **Client** has the right to use these documents for similar projects.”*

7) The agreement (prepared by the consultant) clearly expresses that the consultant retains the rights to the documentation and files, with the client receiving a "permanent non-exclusive, royalty-free licence" to use any patentable processes that are prepared through the project, however, only for the "life of the Project." Of note, in the clause below, the consultant explicitly states that the electronic files cannot be guaranteed or retransmitted, and remain the property of the consultant.

   *"Documents: All documents prepared by **Consultant** or on behalf of **Consultant** in connection with an Individual Task Order are instruments of service for the execution of the Project. **Consultant** retains the property and copyright in these documents, whether the Project is executed or not. Payment to **Consultant** of the compensation prescribed in this agreement shall be a condition precedent to the **Client's** right to use documentation prepared by **Consultant**. These documents may not be used for any other purpose without the prior written agreement of **Consultant**. The **Client** shall have a permanent non-exclusive, royalty-free licence to use any concept, product or process which is patentable or capable of trademark, produced by or resulting from the services rendered by **Consultant** in connection with the Project, for the life of the Project. The **Client** shall not use, infringe upon or appropriate such concepts, products or processes without the express written agreement of **Consultant**. In the event **Consultant's** documents are subsequently reused or modified in any material respect without the prior consent of **Consultant**, the **Client** agrees to indemnify **Consultant** from any claims advanced on account of said reuse or modification.*

   ***Consultant** cannot guarantee the authenticity, integrity or completeness of data files supplied in electronic format ("Electronic Files"). **Client** shall release, indemnify, and hold **Consultant**, its officers, employees, consultants, and agents harmless from any claims or damages arising from the use of Electronic Files. Electronic files will not contain stamps or seals, remain the property of **Consultant**, are not to be used for any purpose other than that for which they were transmitted, and are not to be retransmitted to a third party without **Consultant's** written consent."*

Clearly, the first two approaches, as well as the last approach (the seventh one), are largely unacceptable to any public sector agency looking to retain models for future use within the organisation. The third and fourth approaches reflect an improvement, but there is still room to better convey to the consulting community at the onset of a modelling study, the idea that the model is not considered a one-time use model, but rather is to be used over the long term. The fifth and sixth approaches would have to be altered or adjusted to ensure the ability to use the model in the longer term.

It should be pointed out here that the transfer of the intellectual property rights to the public sector agency is in no way an attempt to prevent the consultants from using and building upon the knowledge base that has been learned over the course of a modelling project and captured into the electronic modelling files. As an example, if the modelling project reveals geological, hydrogeological, or other scientific insights that provide the consultant with knowledge that is marketable to other clients, then certainly it would not be the intent of any public sector agency to prevent these insights from being passed on in other projects. Such insights would, of course, be expected to be disclosed in the documentation that accompanies the model.

4.2.3 New Modelling Studies

When commissioning a new model study it is critical that the ownership/rights to the future use of the model be carefully considered and, if warranted (i.e., model is intended for longer term and for multiple uses), transferred to the public sector agency. There are two main ways in which this can be done:

1) Directly within a legal contract document between the public sector agency and the successful consultant. The contract would be prepared by the public sector agency once the tender for the modelling project had been awarded to the consultant. The contract would be signed by both the consultant and the public sector agency at the start of the project.
2) Clearly stipulated as a requirement of the modelling project within the Request for Proposal (RFP) document – ideally the RFP and the winning consultant proposal should be incorporated as schedules or appendices to any legal contract document that is prepared for the modelling project.

Other ownership options can be considered if they prove to be in the interests of both parties.

Where more than one agency has been involved in the commissioning of a modelling study there are two ownership pathways that could be considered at the onset of the study:

- **Ownership is held jointly by the partnership** – in this case the model would be owned by all the public sector agencies through a partnership agreement. Decisions on the future uses of the model would have to be agreed to by the partnership (i.e., all of the agencies).
- **Ownership is held equally by each public sector agency** – in this case the model is owned equally by each public sector agency in the partnership. Any agency can make use of the model for future studies without necessarily getting approval or acceptance from the other agencies. This is an important point for all partnered agencies to understand. For example, in the future there could be disagreement between agencies as to whether the model is suited for certain types of analyses, however, each agency has the right to make use of the model as they wish. In such cases, the use of the model by one agency may have the potential to compromise work or policies that are in place at an adjacent agency.

4.3 CUSTODIANSHIP

Although any one public sector agency could be the owner of a numerical model, it could be the case that they are ill-suited to playing the role of the model custodian. In this discussion, the model custodian would be the agency or consulting firm who would take receipt of the numerical model once it was finalised at the completion of the modelling study. In the case of the Oak Ridges Moraine Groundwater Program, the YPDT-CAMC (York, Peel, Durham, and Toronto and Conservation Authorities Moraine Coalition) group is currently recognised as the custodian of the many water budget models that have been built in recent years, and that experience is reflected in this document.

A model custodian is anticipated to have strong numerical modelling skills and would exercise several responsibilities at the completion of a modelling study. Broadly, these include:

1) Receive the deliverables of the modelling study:
    a) collect all files needed to run the numerical model from the consultant; and
    b) ensure that the files provided reproduce the documentation provided by the consultant;
2) Archive/store the model files:
    a) establish a server location where the modelling files can be stored; and
    b) organise and store the files for future retrieval;
3) Circulate the model files – transfer the modelling files to agencies/consultants whenever the model is required for future work;
4) Oversee updated model versions – as appropriate, establish procedures/routines for taking back revised model files and for tracking changes from original model;
5) Manage communication – inform all agencies involved as to the status of the model as the above tasks are undertaken;
6) Provide expertise – custodians can provide technical input/expertise to future modelling studies:
    a) advise agencies on the study design;
    b) review RFPs and proposals; and
    c) contribute as advisors over the course of the modelling study.

4.3.1 New Modelling Studies

It is recommended that, right at the RFP stage of the modelling study, an agency/consulting firm be appointed/retained as the long-term model custodian. The designation of a model custodian early in the modelling study will enable custodian staff to be actively engaged in the model study as it progresses, thus ensuring regular contact with the modelling consultant to ease the transition of the model files at the completion of the study. Overseeing the longer term management of the model is a significant task and must be assigned with considerable forethought. Considerations that should be factored into the decision of the best agency/consulting firm to retain custodianship of the model include:

- general strength of the proposed custodian’s information technology capacities (technical skills, customer service attitude, server capabilities, familiarity with model files, etc.);
- technical modelling abilities of proposed custodian’s water managers and technical staff (ability to understand, run, verify, and change a model; ability to manage database files that accompany a model);
- financial strength of the proposed custodian and their ability to allocate (and raise) funds over the long-term to maintain the model (including licence fees for commercial model codes and annual fees for technical support); and
- history as a good steward who has protected the interest of the general public, and has proven an ability to promote accountability and make numerical models accessible for scrutiny, updating, or repurposing.

4.3.2 Existing Modelling Studies

In cases where it has been determined that the model (or selected model components) should be maintained for future use, two steps are recommended:

- confirm that ownership has been transferred (either through the RFP, legal contract, or subsequent post-model agreement) from the consultant to the public sector agency; and
- select the best agency/consulting firm to take on the role of the model custodian, taking into account the considerations mentioned above for new models.

4.4 Updating Numerical Models

Public sector agencies need to improve the reusability, transparency, and knowledge transfer associated with numerical models. However, the updating of a model requires thoughtful deliberation as how best to proceed. Elements of an update can include any aspect of the modelling process that leads to the final model output including: the data used for the modelling study; the storage of this data; the version of the model code; refinement of the conceptualisation of the system; methods applied to evaluate the model; and/or additional processes that are deemed relevant due to new knowledge and information. There are generally three ways in which models can be updated:

1) **On a continual basis** – in practice, models (or their components [e.g., database, geological layering, etc.]) might be updated on a regular informal basis by technical staff, however, it is recommended that widespread access to incrementally updated modelling be restricted and that any informally updated model not be used in an official decision-making capacity. In general cases, only upon returning to the larger policy cycle, as outlined in Section 3, would all incremental changes be captured, tested, peer reviewed, and integrated into a new official model that can then be stamped with a version code (e.g., Version 1.2, etc.) and made available for wider distribution.
2) **On a demand driven basis** (e.g., driven by the installation of a new municipal well, significant updates to model code, etc.) – for models that are updated on an intermediate basis (either regularly or based on demand), once an update has been implemented, these models should be subjected to a rigorous quality assurance/quality control process, after which they can be considered to be officially updated and assigned a version code.
3) **On a regular interval basis** (e.g., every five years) – see comments above.

It is recommended that as models are updated into the future, they periodically be assigned an official version code (e.g., Version 1.2, Version 2, etc.). This allows agencies to keep track of the decisions that have been made through each version of the model. An institutional mechanism that allows for quicker model reviews and updates could be considered to address cases that demonstrate the potential for imminent danger to the general public, for example, as a consequence of a technical error/omission or new information.

For official decision-making that is based on numerical modelling, it is generally recommended that public sector agencies follow on the path of municipal planners in how they address Official Plans (OPs). Municipal planners prepare an OP that is ultimately approved by the Province prior to it taking effect.

On a regular basis (currently every five to ten years) the OP is updated and municipal decision-making is then directed by policies in the new OP. In the intervening years between OP updates, decision-making is based on the currently approved OP. If citizens have concerns with the OP between updates, they can file for an OP Amendment, a restricted change to the OP that, if agreed to, becomes official policy of the municipality.

In a similar manner, decision-making based on a numerical model would rely upon the currently approved official model. However, legitimate questions could be raised as to the scientific validity of the current numerical model (e.g., based on the incorporation of new drilling data into the model and its impact on land use designations or planning). In cases like this, where the model has an impact on land use designations or planning, an application could be made to locally update or patch the model using the new information. Revised decisions could then be made based upon the updated model.

The above is all generally straightforward with respect to future decision-making. However, it is not straightforward as to how to decide whether decisions made in the past should be revisited – or not – based on an updated model. Aspects that should be considered include:

- the risk posed to the general public if decisions based on a model that used out-dated information or methodologies are allowed to remain;
- the public liability tied to revised decision-making based on updated models (e.g., changing drinking water source protection zones may impact new properties and could revise land development approvals; multiple changes over years can be expected and must be conveyed to the general public);
- conversely, the public liability tied to decisions that were made based on a model that used out-dated information or methodologies.

A critical point to consider in determining whether model-based decisions/policies should be updated is the fact the hydrological system is natural and dynamic and therefore can change considerably based on factors such as: i) new climatic inputs; ii) new land development, which in turn may influence runoff, erosion, and groundwater recharge; and/or iii) new and differing water use scenarios. As a result, despite the concern and difficulties with having policy areas change as models are revised, it may prove negligent for a municipality not to revisit and understand any policy changes arising from the use of updated models, and to communicate new insights to the affected public.

One example is updating the mapping of floodplains. There are several reasons why floodplain boundaries could change (e.g., climate change and/or upstream land use change may alter flooding statistics, a review of the original modelling studies may indicate flaws with respect to modern modelling standards, etc.) What happens if new information indicates that a floodplain should be extended? Should historic land development approvals be revised or rescinded? Should information be made available to buyers in the case of a property transfer? What about implications for insurance costs? Can land development approvals be amended after the fact in response to the revised risk exposure, in order to protect the general public? Consider an example where toxic chemicals may be inadequately stored in a newly designated floodplain. Policy amendments, based on the newly delineated floodplain, may prescribe new construction measures, or simply require demonstration of an adequate insurance policy that addresses the revised level of risk exposure, leaving technical details to the market. What are the legalities and liabilities associated with these amendments? On the other hand, what liabilities will a public sector agency face if new information is available but not acted upon?

Another example is the numerical model–driven delineation of source water protection areas. In these areas, policies are increasingly restrictive the closer a property is to a municipal well or intake. If updated model results indicate that lower risk areas (e.g., wellhead protection area [WHPA]-C and WHPA-D, or intake protection zone [IPZ]-2) are in need of revisions, then updating these protection areas will have a moderate or low impact on property owners, and the changed risk to the public will equally be moderate or low. However, if models indicate shortcomings in the delineation of higher risk areas (e.g., WHPA-B), then updates to these areas may significantly impact property owners but also reduce the risk to the public significantly. Case-by-case assessment of the costs and benefits of updating source water protection areas may be required. Given the uncertainty associated with the modelling, and taking a precautionary approach, it may be appropriate to only expand capture zones as models are rerun and results are refined; that is, the WHPAs would never be refined to be smaller in area. This would tend to eliminate concerns amongst technical staff that land parcels may be initially designated as lying within a WHPA, then possibly removed with a model update, and then again possibly re-designated, perhaps owing to changes in pumping schedules. This type of back and forth approach could considerably affect the confidence that the public places in the scientific process of assessing the groundwater system through modelling. Another approach to address the uncertainty associated with this issue was taken in the Region of Waterloo, where capture zone 'envelopes' were created using three or four different, fully calibrated models, where key parameters (e.g., vertical transmissivity, porosity, etc.) were adjusted within reasonable ranges. This resulted in the delineation of multiple capture zones, all of which were amalgamated to derive a robust, conservative, capture zone 'envelope' that was eventually used for official plan policies.

These two examples highlight procedural challenges of implementing cyclic or adaptive water resources management. Much research is needed regarding the evolution of public agencies to agencies that are permanently learning and adapting their decisions to changing environmental conditions, public risk and perception of risk, changing liability regulations, and an expanding knowledge base. For many decades, planning procedures have been thought of as being fairly static since, from a governance perspective, it is not practical to frequently revise, shrink, and expand designated planning areas. However, the above examples demonstrate that model results can change with changing environmental conditions. How can agencies act upon new insights, while balancing their mandate to, on the one hand, protect the public, against, on the other hand, liability claims by property owners? How can planning procedures be better designed to support regular adaptation or updates? These fundamental governance questions require additional guidance given the legal uncertainty surrounding the concept of changing policy area delineations.

For now, agencies are encouraged to incorporate new data/knowledge/insights that are brought forward through model sharing with external parties. All updates coming back to the agency should be collected and incorporated into the agency's updated official model. It is also important to consider that different elements of a model (e.g., database, conceptualisation, parameterisation, etc.) can be updated independently from other elements. The periodic updating of official models allows for each independently updated element to be brought together through an updated versioning system.

4.5 DATA SHARING

Ontario's water managers are finding themselves working in an era of change as a new water management regime unfolds. This new era is seeing numerical modelling as a commonly used tool for understanding, analysing, and ultimately making decisions with respect to water resources. As a result, it is now incumbent upon public sector agencies to have rigorous data management systems in place, for it is this data upon which numerical models are based. The days of orphaned Microsoft® Excel® files being abandoned on computers upon staff turnovers should be drawing to a close.

All agencies that have commissioned modelling studies must review and understand the data upon which their numerical models are based. In ideal situations, all models that are under the purview of one agency would have been constructed using a central database, which is actively managed and updated by the agency. This is the recommended best practice for all agencies. In other cases, the consultant might have assembled the required data upon which each model was based. Where numerical model boundaries cross agency boundaries, the consultant might have acquired the data from more than one agency and assembled or merged it into a new combined database. If no central actively managed database is made available, then consulting fees for data assembly will be incurred by the agency.

In the case of the 13 partnered agencies that manage the geographic area covered by the Oak Ridges Moraine Groundwater Program, the program provides an overall data management infrastructure that can be drawn upon for any numerical groundwater or overland-flow water balance model. The database houses all groundwater well data (e.g., geology, construction, etc.), as well as temporal data (e.g., water levels, water quality, pumping, etc.) associated with the screens at each well. It also contains the locations of surface water and climate stations and the data associated with these stations (e.g., streamflow, precipitation, temperature, etc.). The database is actively managed such that any newly collected data (e.g., data collected as part of a consultant-led modelling study) can be readily imported back into the master database for future use.

A question that has arisen in the sharing of an agency's database is one of knowing who is making use of the database and for what purpose. Conservation authority and municipal government agencies are generally open to sharing databases since it fosters increased knowledge, can lead to database improvements (e.g., error correction), and ultimately leads to better decision-making. However, agencies in the past have commonly required the signing of data sharing agreements simply so they know which studies the data are being applied towards and how the data are being used. This prevents unwanted surprises, for instance, their own data coming back against them in cases such as development disputes (e.g., Ontario Municipal Board hearings).

In addition, there is a standard of care that is carried out, and expected, with the management of large ongoing databases, however, there can be instances where incorrect data are found within a database. Therefore, agencies must be diligent in preparing disclaimers, reminding users of their responsibility to use the database with care, and routinely checking the database.

The following points are key considerations for data management at public sector agencies:

- Data management can no longer be considered a non-core business function of the organisation, indeed it is key to readying organisations for a strong future with numerical modelling.
- Processes must be put in place to efficiently move new data into its right place in the database (e.g., digital forms that help with data input and importing).
- All agency technical staff must have a data management focus to their work, for example, staff coming across new information in the course of their day-to-day work should immediately be thinking of the most effective way to capture data and where it should be stored. As well, there should be readily available methodologies on their computers to effectively facilitate such data capture.
- Agency staff must also pursue regular database management training to ensure best management practices are being followed.
- Projects tendered out to consultants must explicitly express the need for effective capture and incorporation of new data into the agency's data management structure. This removes complications with respect to the reproducibility of modelling results by eliminating database divergence, particularly in cases where other consultants may make use of agency databases for future modelling projects.
- In cases where consultants take a corporate database for the purposes of building a numerical model, there must be requirements that new and/or changed/corrected data be returned upon completion of the project. This data should be returned in a format that can be readily re-incorporated back into the agency's master database.
- Given the large amount of time necessary to effectively manage databases, it is encouraged that, where feasible, agencies partner to create larger more effectively organised and managed databases. The Oak Ridges Moraine Groundwater Program (formerly known as YPDT-CAMC Groundwater Management Program) is one effective example of such a partnership.
- Data sharing is encouraged but the signing of a simple data sharing agreement (see Appendix 3 for examples) is recommended. It is important for longer term open data sharing that municipalities and conservation authorities not be unduly surprised when their own data are used in cases where they might be in opposition to a proponent. The signing of a data sharing agreement should not be a hindrance to data sharing and agencies should have processes in place to efficiently process such agreements.
- Disclaimers must be put in place to indemnify agencies of misinterpretations caused by erroneous data or misuse of data (see Appendix 3 for an example).

4.6 Model Sharing

For both new modelling studies and existing models, model accessibility or sharing is an issue that is best addressed as early as possible. For existing models, this issue has typically not been addressed in any meaningful way and agencies are left with no direction as to how best proceed when a model sharing request is made. It is recommended that generalised model sharing policies be agreed upon by agencies involved in a modelling project such that all parties have a good understanding as to the response they can deliver when an inquiry is made. Within the agreed-upon model-sharing framework, details on model sharing would be determined on a case-by-case basis between owners and custodians.

In all cases where a model owner is requested for access to a model, it is recommended that the owner ask for details as to how they propose to use the model. This provides the model owner with a sense of how appropriate the model might be for the intended task as well as to whether the information garnered from the use of the model might be worthwhile to re-incorporate back into an updated official model.

The following aspects need to be considered when it comes to sharing a technical model with others:

1) whether the model should be shared and whether the model should only be shared with parties that meet certain requirements;
2) how to word the disclaimer that indemnifies the owner and all employees from any liability that might be associated with model sharing;
3) whether (and how) any new insights/data should be communicated back to the model owner in order to improve upon the official model;
4) who will own any products derived from the original model, and any intellectual property rights that a secondary user derives from their modifications;[7] and
5) how will the original model be referenced, particularly in cases where it has been altered.

Many of these issues can be addressed in a Model Sharing Agreement, an example of which can be found in Appendix 3.

There are several key advantages to making a model accessible to other practitioners:

- sharing is a precondition for independent review, which enhances the interpretation/understanding of the study system;
- decisions built on model results become more accountable, transparent, and arguably in the best interests of society as the model gains widespread use;
- models prepared by public sector agencies are typically paid for through public funds, therefore, making the models accessible to others ensures efficient use of limited resources; and
- practitioners can build on and continuously improve a single consistent model, rather than having to ‘reinvent the wheel’, possibly repeating errors.

In a collaborative manner, all users then benefit from the improved knowledge and data.

From an individual agency point of view, there are several disadvantages for sharing models, however, many of them can be addressed through well executed model management practices. Improved model management of course comes with additional costs in terms of staffing, and these costs would have to be balanced against the potential gains in terms of system understanding through model sharing.

[7] For example, a GNU General Public License agreement (Free Software Foundation, Inc., 2007) guarantees end users the freedoms to run, study, share (copy), and modify the model, but also protects the intellectual property rights of the original owner.

One immediate concern associated with model sharing is public security (e.g., if the model points at a high-risk location where drinking water sources could be intentionally polluted). Several other concerns include:

- inadequate capacity of agency staff both from a technical and time commitment view to assist a consultant, especially in cases where technical capacity is lacking at a consulting firm (a custodian may be able to assist);
- inadequate legal guidance on liability (hence a strong standardised disclaimer is recommended);
- inadequate documentation of the model alterations by the user (hence the recommendation that model users include sufficient technical details on the full modelling process); and
- the potential for the model to simulate system processes that were never considered during the original model development, and thus the model may not provide defensible results.

The above concerns also suggest that it may not be feasible to share every model immediately. Instead, guidance on disclaimers and other legal aspects are required, as well as a minimum quality assurance process based on robust criteria, in order to ensure that public agencies demonstrate adequate technical standards.

4.6.1 Return of Updates Tied to Model Sharing

As the model owner, agencies have a wide spectrum of opportunities in how they address the question of whether to accept changes to the model or elements of the model. Model owners can develop blanket policies that either require all model users to share back their revised model (or its elements) or never require the submission of model updates. However, it will likely be that model owners determine this on a case-by-case basis. Within a model sharing agreement, owners could take the position that they maintain the right to request that a revised final model (or model elements) be returned. They can then meet with the user of the model to judge as to whether there have been any significant insights or new understandings added to the model. Based on the meeting, the model owner can at that time decide whether or not to act upon the right to take back an updated model (or model elements). It might be in the interest of the model owner to establish either a technical committee or a more rigorous/formalised process to determine whether changes to a model by external users merit incorporation back into the official model. Some of the considerations that should be evaluated when making this determination include:

- the staff time and financial capacity required to incorporate any new information into the original model;
- the likelihood that the information will significantly alter results, policies, and/or decisions made using the existing model;
- the magnitude of the model update versus the entire model area (e.g., did the model update only affect a local area within a regional model?);
- the reliability/quality of the information that will be returned by the user; and
- the magnitude of new data incorporated into the updated model.

Consideration can also be given to accepting some of the model files. It should almost always be the case that the use of a model require the delivery of any new data back to the database (i.e., data confidentiality claims are not accepted as reasons for non-delivery of data that may change the model, however, the decision to require the delivery of interpreted files could depend upon the significance of the changes made to the original files).

4.6.2 Liability and Disclaimers for Model Sharing

Model owners that are willing to share models must take precautions to ensure that they are not held liable for decisions that are made by a model user. Model sharing agreements must incorporate liability/disclaimer clauses that will ensure that the model is transferred with the model owner accepting no responsibility for model-supported decisions made by the model user. An example of a disclaimer from the National Research Council of Canada (National Research Council of Canada, 2016) is presented in the inset box. Appendix 3 also provides a more generic disclaimer that can be incorporated into a model sharing agreement.

4.7 TECHNICAL CAPACITY OF STAFF

Certainly, a large part of the unpreparedness of public sector agencies to effectively embrace numerical modelling, as mentioned above, is tied to the technical capacity of staff. In Ontario, numerical modelling has quickly evolved from the late 1990s and early 2000s when steady-state equilibrium models (albeit fairly complex and regional-scaled models) were first being used in the realm of groundwater hydrology. Today, numerical modelling has evolved so that groundwater is fully transient and fully integrated with surface water. These newest models are highly complex and take considerable skill to effectively run, evaluate, and interpret the results. Technical capabilities at every level of government (federal, provincial, municipal, and conservation authority), and indeed at many consulting firms as well, have simply not kept pace with these technical advances.

Given this reality of limited technical capacity in numerical modelling, one of the most effective ways for public sector agencies to move forward is to share staff resources to build a richer numerical modelling talent base (i.e., increased number of individuals with modelling skills as well as increasing the skills of those individuals).

EXAMPLE OF DISCLAIMER FROM NATIONAL RESEARCH COUNCIL OF CANADA

5.0 Limited Warranty (as adapted from National Research Council of Canada, 2016)

5.1 "Model Owner" does not warrant the model or any associated software to be correct, free from defects, suitable for any purpose, or compatible with any model or computer.

5.2 Because the model is inherently complex, it is the Licensee's responsibility to verify the model or any associated software and any work produced using these. "Model Owner" rejects all liability and responsibility relating to the consequences of using the model. In no event will "Model Owner" be liable for indirect, incidental, economic or consequential damages arising out of the use of the Software, including, without limitation, damages or costs relating to loss of revenue or profits, business, goodwill, data or computer programs, or claims by a third party. Except for representations and warranties expressly made in this Agreement, the model is provided on an "as is" basis, and there are no representations or warranties, express or implied by statute, including, without limitation, any with respect to:

a) Merchantability or fitness for any purpose;
b) Operational state, character, quality or freedom from defects.

5.3 The Licensee shall indemnify and save harmless "Model Owner", their employees and agents from and against, and be responsible for:

a) All claims, demands, losses, damages, costs including solicitor and client costs, actions, suits or proceedings brought by any third party, that are in any manner based upon, arising out of, related to, occasioned by, or attributable to the use of the Software
b) Other costs, including extra-judicial costs, of "Model Owner" defending any such action or proceeding, which "Model Owner" shall have the right to defend with counsel of their choice.

5.4 "Model Owner" has not knowingly infringed on any copyright. If the Licensee receives or becomes aware of any claim or assertion by a third party that the model licensed under this Agreement constitutes an infringement or other violation of third party's patents or other intellectual property, the Licensee shall notify "Model Owner" and shall provide "Model Owner" with all the details relating to the allegation, within 15 days of its knowledge of the allegation. "Model Owner" shall promptly enter into discussions with the third party to obtain any additional rights required, such as may arise if a third party's patent emerges. If necessary rights are not obtainable on commercially reasonable terms, "Model Owner" agrees to cancel the licensing agreement if requested by the Licensee.

It is recommended that any Ontario public sector agency who has commissioned a numerical modelling study over the past decade take an inventory of their staff's abilities to effectively run and interpret the agency's model(s). It may be that the capacity is sufficient or that there is sufficient funding to either further train their own staff or to retain consultants to act on their behalf. However, where capacity is limited, this may warrant a frank discussion with adjacent agencies to see whether a joint arrangement can be made to retain technical modelling capacity.

A key point to highlight in moving forward with numerical models, is the fact that one of the most important requirements in moving forward to successfully use models is a skilled modeller.

THE OAK RIDGES MORAINE GROUNDWATER PROGRAM AS A SUCCESSFUL EXAMPLE OF COLLABORATION

The Oak Ridges Moraine Groundwater Program (ORMGP; formerly known as YPDT-CAMC Groundwater Management Program) provides an example of many public sector agencies (in this case, 13 agencies) partnering to share expertise by creating an informal centre of excellence. Formally established with the hiring of a program manager in 2001, the program has evolved to become a small group of reliable technical experts with expertise in data management, geological and hydrogeological interpretation, and, more recently, in numerical modelling. Since 2006, there have been numerous numerical models created within the partnership area. In 2013, it was quickly becoming evident that the knowledge gained through these modelling studies would be in jeopardy of being lost or ‘shelved’ given the lack of numerical modelling expertise. Partner agencies agreed to fund a joint position (an expert modeller) through the program in order to better capitalise on the investments that had been made in numerical modelling. This has enabled the program to establish itself as the custodian for the many numerical models that have been commissioned through the individual partner agencies. As custodian for the models, staff have built experience in model management as presented throughout this guide.

The ORMGP provides a concrete example of how agencies in other parts of the province can move forward to embrace the challenge posed by the technical advances that numerical modelling presents to water managers.

5 MODEL DEVELOPMENT AND CUSTODIANSHIP PLAN

This section discusses the requirements and expectations that project managers should consider prior to, during, and subsequent to a model development study, and, in addition, describes the data needs that modelling consultants require in order to undertake modelling studies.

The discussion that follows is built upon the experiences gained through the Oak Ridges Moraine Groundwater Program (ORMGP), which, following the source water protection (SWP) program, has accepted custodianship of over 50 regional-scale groundwater and overland-flow numerical models from its 13 partner agencies. None of the partner agencies had the capacity to fully review or utilise the models, so collectively, a joint model custodianship program was established under the umbrella of the ORMGP.

In order to successfully take responsibility for the eventual custodianship of a numerical model, it is important for the model custodian to understand how models have been constructed. In circumstances where a model is just being newly constructed, it is ideal to incorporate into the role of the model custodian the steering of the modelling study to ensure that the numerical model is built in a structured manner following a set of best practices as outlined within this section. Even though many of these practices, discussed below, are focussed on aspects related to the development or building of a numerical model, they constitute, together with the longer term aspects of managing numerical models for longer term use, an integral part of a long-term numerical model custodianship plan.

The ORMGP model custodianship program was designed such that the model file storage aligned with the model development workflow process, both conceptually and chronologically. This custodianship scheme was chosen to both assist in organising existing numerical models as well as to instill a best management practice for new and/or refined numerical modelling products. The overall design objective was to standardise and simplify future modelling efforts in order to:

1) ensure adequate data preparation prior to the start of a project, thus promoting efficient data exchange;
2) foster ongoing engagement between agencies and consultants through the use of progress logs to document model development;
3) ensure reproducibility of results for review and quality assurance;
4) guarantee completeness of project deliverables thereby reducing potential entry barriers for future model users;
5) standardise file storage, accomplished by prescribing a standardised file structure; and
6) simplify model transfer and redistribution for future projects, accomplished by prescribing independent model storage locations on the server.

The program goal is to maintain a management system that captures digital numerical modelling files. The program is also set-up to provide complete documentation of current and future model refinements, and the digital recapturing of refinements to modelling files, following along a progressive path of knowledge building. This provides an effective means for Ontario’s public sector agencies to obtain future utility from past modelling efforts. Recognising that model development is a continual and iterative process, the custodianship program described here aims to foster the re-use of models and/or model elements/components.

5.1 WHEN IS MODELLING REQUIRED?

Before engaging in any hydrological modelling study, public sector agencies are well advised to consider whether a model is the best tool to address the issue and, if so, what level and scope of modelling is best suited. Questions that help to direct this decision can be grouped into five categories:

1) Study purpose and requirements:
    - What is the purpose of the analysis and could it include modelling?
    - What are the legal/legislative requirements for modelling?
    - What is the simplest form of modelling that fulfills this requirement?
    - Are there options other than modelling?
2) Assessment of technical expertise:
    - What technical expertise is available for:
        - supervising a consultant-led modelling study?
        - defining the modelling scope?
        - specifying Request for Proposals (RFPs) and contracts?
        - reviewing proposals both scientifically and administratively?
        - aggregating input data?
        - performing additional monitoring?
        - communicating project progress?
        - reviewing model deliverables?
    - Alternatively to a consultant-led study, is there technical expertise available to undertake a modelling study internally within the agency?
    - Is technical expertise available to perform basic updates or variations of analysis using an existing model?
3) Assessment of existing models:
    - Are relevant models or model components already available in the study area that can be applied to the study?
    - Is there a potential to use an existing model(s) to investigate the questions of interest?
4) Data availability:
    - Are data available for the proposed modelling?
    - What additional data would be required in order to meet the intended purpose?
5) Budgeting for a modelling study:
    - Is there sufficient funding available for the proposed study?
    - What is an expected time-frame for the proposed study?
    - What are the consequences if the modelling study takes longer than expected?

A prime objective of a model custodianship program is to help leverage existing model-related investments toward future water resources–related knowledge capture and model improvement. As the above questions are being considered, the model custodian (should one have been identified and available) is the person most familiar with all elements of the existing models, and is in the best position and best qualified to help.

To maximise the effectiveness of any model custodianship program, it is recommended that model custodians be fully engaged in future model-related decisions, particularly at the scoping stage of future modelling studies since this is when the crucial decision as to whether to use an existing model or to build a new model takes place. If it is determined that an existing model can be used, then the model custodian can also help agencies determine whether any modifications may be required prior to the re-use of the model.

5.2 PROJECT SCOPING

If numerical modelling is identified as the appropriate means to address an issue, then a project scoping step is recommended prior to the issuing of an RFP to the consulting community. The scoping step is intended to: i) define the project objective(s); ii) specify realistic expectations from the proposed numerical model, within the available budget; and iii) prepare all information that a modelling consultant will require. An adequate scoping study significantly reduces the risk of future changes to the scope of the model study, overruns in costs and time, and model results that are not well aligned with the model study objectives.

Once the project objectives are clearly defined, the expectations must also be clearly outlined so that they can be conveyed to consultants within the RFP. Agency staff must be careful in trying to match their expectations from a numerical modelling study with the budget available for the study. The following questions can assist in arriving at reasonable numerical modelling expectations:

- Is there a clear and consistent understanding/expectation of the results/output of the proposed modelling exercise both from technical and managerial staff?
- Can the expectations be presented within the RFP in a concise manner that is void of ambiguities, which may be misinterpreted by a consulting firm?
- Do agency staff have a clear understanding of the uncertainty and limitations expected with the model results?
- If the modelling exercise is unable to meet expectations (e.g., due to data limitations, timelines, data access issues, model capability, computer/technology limitations, large uncertainty, etc.), is this an acceptable outcome? Can the project be delayed to meet expectations?

Similarly, when considering the data that has to be assembled for the modelling study, the following points/questions can provide guidance:

- Are data available in-house or through other public agencies?
- Are there existing models with data sets available in-house or through partner agencies?
- Is there an intention to have a consultant compile the data?
- What if the required data are unavailable or of poor quality? Should:
    - the project timeline and cost be extended in order to collect the required data?
    - the project scope, or agency expectations, be adjusted?

- a modelling approach be abandoned?

- In order to minimise project cost overruns and poor quality results as much as possible, deficiencies in data should be identified and addressed by agency staff prior to RFP preparation. If necessary, data assembly could be prepared by a different consultant prior to modelling.
- Does the modelling involve hypothetical scenarios to be modelled? If so, are the required data readily available to run the scenarios (e.g., future development plans, climate change projected weather patterns, etc.)?

Generally, public sector agencies have greater access to background data and information (e.g., geospatial data, future land use planning, monitoring data, pre-existing studies and models, etc.) than do consulting firms. As part of the scoping step, agency staff must take full responsibility for data assembly and organisation to ensure that data are in the best shape possible (e.g., current, standard format, quality assured, etc.) prior to contracting modelling work. Experience has demonstrated that when organising available data, significant data inadequacies and gaps are frequently discovered. If not undertaken prior to the retaining of a consultant, these data gaps are uncovered during the model development phase resulting in costly modelling delays. In many such cases, a contingency plan has to be initiated that tends to increase costs while failing to attain the anticipated results.

It should also be kept in mind that poor data quality may not be discovered unless applied in a modelling framework. Standard automated data quality assurance tools can never be perfect, and as a result data delivered to consultants may be found to be erroneous.

Project scoping requires modelling expertise. This could come from staff, a custodian, local experts, and/or independent consultants. Should there be some uncertainty as to how a modelling project should proceed, it may prove worthwhile and cost-effective for an agency to consider releasing an Expression of Interest (EOI) document to the consulting community to solicit additional guidance. This process should, at a minimum, help in determining the type of modelling required to address the issue at hand. From there, the requirements of such a model would still need to be determined.

At the completion of the scoping step, agency staff should have a clear understanding of their expectations from the proposed modelling study as well as their situation with respect to the data needs. All available data sets will have been reviewed for quality, and it will be confirmed that the data are sufficient to inform/guide/constrain the project. There may be cases where the approach is further informed by consultant proposals and/or EOIs. Issues may be raised that were not previously considered.

5.3 Request for Proposals

The next step is to issue an RFP to the consulting community to solicit bids for the required work. The above scoping step will allow for a clear, concise, and descriptive RFP to be written, and will help to make the review of the bid documents straightforward. This will expedite the start of the project.

At the RFP stage, agencies must have an idea of the funds available to complete the modelling study (the costs should have been taken into account during the scoping step). Typically agencies do not disclose the amount of funding that is available for any given study in hopes that the proposals coming in from an RFP will prove lower than anticipated. This is certainly an option that can be used for modelling projects. However, given the propensity of modelling projects to run over budget, consideration should be given to disclosing the available funds within the RFP. The advantage being that it conveys to the consulting community the level of modelling effort that is expected by the client. If the costs are divulged then the RFP can be tailored to solicit the highest technical level of modelling for the allocated funds. This allows consultants to gauge the amount of effort that is expected and whether the project scope and expectations are reasonable. Consultants could at this point choose to bid on the project as presented or they could choose to strategically target key components of the agency's modelling goals and adjust their proposals to provide the most cost-effective analysis. Agencies should also consider reserving a portion of the allocated funding in anticipation of unforeseen issues that would require additional time and money.

It is important that the RFP clearly and concisely lay out project goals, all data that will be provided, and expected deliverables. A sample RFP is provided in Appendix 3, however, an RFP needs to be tailored specifically to the modelling scope and data requirements will be dependent on the type of model being used. Jenkinson (2012, p.9) also emphasises that the following be considered when preparing an RFP:

1) the issues that require action and the project objectives;
2) the engineering and scientific requirements or deliverables of the study (such as temporal and spatial resolution, the processes represented, dimensionality, speed of data availability, and the capabilities of the model to handle available input data and provide useful output data formats);
3) the specific communication deliverables of the study;
4) a detailed stewardship plan;
5) a socio-political impacts statement; and
6) the resources and costs required to complete the study.

Boorman et al. (2007) points out that technical modelling knowledge (e.g., provided by the model custodian) be brought into preparing the RFP because issues that appear to be obstacles to the non-expert may actually be resolved at very low cost by expert knowledge and insight.

5.3.1 Project Expectations

Any RFP should begin with a clear description of the problem that is being addressed and the modelling objectives. It is often helpful to frame the objectives through a well-defined project scope/hypothesis test. The clarity in which the expectations are described can be paramount in leading to a successful modelling study.

Expectations should also include any proposed model scenarios (where applicable). In planning scenarios, agency staff should keep in mind that:

- scenarios tend to be multiplicative and could significantly add costs to the project (e.g., 3 climate states [i.e., current, drought, flood] x 3 land use states [i.e., past, present, future] x 4 watersheds requiring water budget computations equals 36 model runs, and could require separate discussions of the 36 model results); and

- scenarios will generally require an additional baseline scenario for comparison, which could be considered the calibrated model or simply an additional model scenario (e.g., pre-development conditions).

It would also prove useful to the consultants bidding on the project, if at this point, the RFP provided some direction on the desired model calibration target(s), the overall modelling objectives, and any strategies that the consultant might consider to ensure that the model is adequate in achieving the set goals. This may be difficult to determine without expert modelling opinion and may have to be reformulated after review of the solicited proposals. Another option is to entertain an EOI prior to the RFP.

The RFP is also a good place to stress the need for the consultant to provide continual engagement and communication. Model progress should be communicated regularly. The RFP should indicate that over the course of the project, consultants, upon becoming aware, notify the client in writing of any arising issues that will cause delays.

5.3.2 Data Expectations

The consultants for whom the agency is soliciting proposals need to know which data are available in order to scope an appropriate plan of action and for budgeting purposes. Consultants deserve full disclosure of data that are available for the modelling project. The RFP should convey whether the data has already been compiled by agency staff (as suggested above) and whether it can be assumed that the data have been checked and are void of error. If the data has been assembled specifically for the project, it would assist the consultants in preparing their proposals if the format of the data (i.e., software specific, file extensions, relational aspects of database, etc.) was also specified in the RFP. The database/data sets could also be made available for review by consultants over the period in which they are preparing their proposals. If the data has not been assembled and is expected as a deliverable of the project, then agency staff should provide an indication of the format in which they would like to receive the data. Data should be delivered between the client and the consultant in standard file formats (see inset box).

In cases where existing models are available and are to be provided, model files being delivered to the consultant need to be defined and can even be made available for review as proposals are being prepared. Relevant project reports that provide background information should be part of this package. Depending on the model code/software package used, model files can come as stand-alone single files or as a set of model files used to specify model input variables, parameters, and model control/specifications. For the latter case, to ensure a complete model file transfer, the model files that should be provided include:

- control files that specify model simulation options (such as model time periods) and are linked to, or point to, model input files, boundary condition and parameter files, and specify the location to write output files;
- parameter files that instruct the model on parameter distribution, boundary conditions, and initial conditions; and

- input variable files, used to specify temporal inputs (i.e., climate data, flow data, water takings, dam operations, etc.).

A quick test to ensure that all model files are accounted for is to simply run the model; if data are missing, the model should not run to completion.

STANDARD FILE FORMATS

- Point time series data (one-dimensional) – as ASCII files (comma-separated or tab-delimited values) and/or database files (*.mdb, *.sql, *.bak). Spreadsheets (i.e., Microsoft® Excel®) should be avoided as they are notorious for being delivered with non-standard formatting and broken links.
- Static (temporally) spatial data (two-dimensional, maps):
    - vector shapefiles (*.shp); note that these require additional accompanying files such as the shape attribute database file (*.dbf) and the shape index file (*.shx)
    - raster files (i.e., grid-based data) – ASCII grid files (*.asc), standard floating-point files (*.flt) and their associated header files (*.hdr)
    - Esri geodatabase file (*.gdb)
- Distributed time series files (in raster format; three-dimensional) – as time-stamped or time-labelled raster files (*.flt, *.asc) or Network Common Data Form files (NetCDF).

5.3.3 Deliverables

The RFP should clearly define the project deliverables to ensure that project expectations are met; this could easily be accomplished in the form of a checklist. Deliverables <u>must</u> include the operational model, which includes all model files. It is recommended that the delivery of the operational model be considered complete when the delivered model files have been demonstrated to have successfully run to completion on an agency workstation and successfully reproduce the delivered model outputs and the results documented in the project report.[8]

The data or files that are expected (e.g., model results, maps, spatial data files, additional measurements, processed/cleaned data, selected model outputs, etc.) should also be specified as deliverables. If complete modelling workflows are described and the reproducibility of the model results is confirmed, then it may not be necessary to provide all model outputs, thus avoiding the delivery of copious amounts of output data. A detailed list of expected model files that could be added to an RFP is given in Appendix 3.

The RFP should also specify that the consultant deliver the model and all associated files to the client via a storage medium that is agreed to by both parties. Options for delivery can include either internet-based (FTP [file transfer protocol], cloud storage) or physical (hard-disk drive [HDD], a solid-state disk [SSD], or a flash drive) options. A good rule of thumb is that internet-based transfers are not advisable if downloading takes more than one work day (eight hours), otherwise a physical delivery is recommended. If it is possible that physical drives may be required for file transfer, it should be specified at the RFP stage so that consultants can budget for them in their proposals.

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[8] Be aware that certain modelling software packages are proprietary and may require a principle fee and annual support fees; other software packages exist that are free and open source.

5.3.4 Model Report

The RFP should provide a clear description of what is expected in the final project report, perhaps even specifying sections to be included, and also what is not wanted (this helps to minimise costs and review time). If the prepared model is designed for longer term water management, then the RFP should specifically request that in the final report the consultant provide comment on the suitability of the model for purposes outside of its original intention and scope.

Another requirement should be that the consultant must clearly communicate modelling workflows for the sake of reproducibility, including:

- data processing steps and methods, including which software tools were used;
- steps and scripts used to generate model input files, model scenarios, and model executions;
- steps and scripts used to evaluate model output files in order to generate results; and
- the model code and all other executables needed to reproduce results.

5.3.5 Intellectual Property

The RFP must include a discussion on intellectual property and how the client agency can access the necessary modelling code and associated software to reproduce results. In order for others to reproduce model results in the future, it is necessary for consultants to disclose all elements of the modelling workflow, including those that may be protected through intellectual property rights. Consultants must provide options to access these elements for independent review and future use or, alternatively, lay out a clear procedure on how model results could be reproduced through independent parties and state the associated costs. As part of model delivery, agency staff and/or the custodian may request additional training to handle the operational model and associated workflow tools. In this case, the RFP may incorporate a request for the consultant to provide training and knowledge transfer.

Unlike projects that deal with physical infrastructure or services, modelling studies often raise questions regarding intellectual property rights. If the agency requires the use of the model for future projects, then assigning intellectual property rights to the agency upon completion of the model must be made clear. All software tools and elements of the modelling workflow that are protected by the consultant’s intellectual property rights need to be listed in their proposal, together with options for accessing these tools; access could be granted through license agreements with the consultant.

Agencies must specify how the consultant can use the model with their other clients, including any model component (e.g., geological layers, future land use/development plans, municipal pumping rates, dam operations, synthesised data, hydraulic conductivity distributions, etc.). It is recommended that the RFP and the legal contract contain a clause stating that future use of the model and any of its components shall be prohibited without the written consent of the agency. A further discussion on this topic along with examples of several legal clauses around ownership/intellectual property rights that can be considered in preparing contract documents is discussed in Section 4.

5.4 Proposal Review and Contract Agreement

With a scoping study and a well drafted RFP, many aspects of the proposal evaluation will be expedited. Evaluating proposals will require in-depth expert knowledge and, if not available internally, it is recommended that agencies consult with their model custodian, academic reviewers, independent consultants, or partner agencies, and perhaps bringing in external technical experts to formally assist with proposal evaluation.

During proposal review, all aspects of the RFP will need to be considered; some shortcomings in proposals may be less relevant than others. Independent reproduction of results should be considered to be of critical importance, for example, to assist in cases of litigation. Proposals that do not ensure a transparent transfer of models and data should be avoided.

After selecting the consulting team whose proposal was found to best meet the selection criteria, a legal contract is drafted. The RFP and the consultant's proposal should both be included as appendices to the legal contract and will form the framework for the work that will be undertaken. The signed contract will demonstrate that both parties have agreed to the terms of the contract and the proposed modelling pathway. The contract can be thought of as a consolidation of RFP requirements and insights from the proposals; there is no place for surprises.

5.5 Project Start-Up

With a signed agreement in place, data can be passed to the consultant, as laid out in the contract and RFP. It is recommended that the consultant be provided an opportunity to review the initially delivered data and that they confirm with the client that the data provided is complete as agreed upon. Once this is agreed to, the technical modelling work begins. Keep in mind that if the agency cannot provide the data as agreed upon in the contract, then the consultant is not legally bound by the timeline of the contract.

If a peer review committee has been commissioned to review the work, it is recommended that they be present at the start-up meeting. Their role must be clearly established and reasonable timelines should be set for their contribution. All three parties, that is the client, the consultant, and the peer review committee, must fully understand (and uphold) their role in order for the committee to prove effective.

5.6 Project Course

All project timelines, including meeting dates and draft report submissions, should follow the schedule agreed upon at project start-up. Any reasons for not meeting deadlines must be documented by the consultant and provided to the agency in a timely manner.

The SWP experience suggests that establishing and maintaining a professional collegial relationship between agency and consultant staff throughout the project is invaluable to the transfer of technical knowledge gained through the model development process.

5.7 PROJECT CLOSURE

At project completion, the model and all model data are delivered according to the contract agreement. Final reports are approved (including by the peer review committee, where applicable) and the consultant provides a presentation to discuss the model findings. The presentation should include some direction from the consultant as to additional work that could improve their analysis or the model in general, and should indicate how these potential improvements were identified and the types of changes in model results that might be expected with these improvements. Other issues, such as possible future training on the use of the model or potential future uses of the model, would also be discussed at this time.

5.7.1 Transfer/Delivery of Model and Data Files

At the completion of a modelling project it is critical that all relevant files be transferred from the consultant to the client agency. The model delivery is a crucial component of any modelling study and, if made properly, the data/results/model(s) will integrate seamlessly into an agency's model custodianship program. File transfer should be undertaken shortly after project completion while the files are still active, easily located, and can be re-copied if found to be corrupt.

It is likely that most municipalities and conservation authorities across Ontario have had some interaction now with numerical modelling. Prior to 2000, in the early days of groundwater modelling, models would have been created as single use models, developed to answer a particular question. There was little thinking as to the longer term use of the model and therefore as how to best manage or share modelling files. As a result it was frequently the case that government agencies had no need to request the modelling files. In rare cases where model file transfer had been requested, it remained difficult to determine whether the delivered model file package was complete and all of the necessary files were transferred. It is now proving costly for public agencies to request the original model files from the consultants who prepared them, in some cases years after a model study has been completed. Consultants must first find the model files, check for completeness, likely by rerunning the model, and then transfer the files. Charges of tens of thousands of dollars have been incurred to undertake such tasks.

Experience has shown that modelling contracts often fail to explicitly require the transfer of numerical modelling files and even in those cases where file transfer has been specified there has rarely been confirmation that the required files were indeed delivered. Experience has also shown that large file transfers run the risk of being corrupted and that files delivered as per the contract can prove to be unreadable. Running the model to completion should therefore be a requirement of file delivery. It is advisable that both the RFP and the legal contract define a file naming convention that is intuitive and self-explanatory. Delivered input files sometimes cannot be readily identified making it difficult or even impossible to reproduce the documented modelling results.

There are several ways to complete the model file transfer and they are listed here in the order of preference:

1) The consultant helps install the modelling software onto the agency's (or the custodian's) computers/servers, running the model to reproduce the results, and delivering basic training on how to execute the model and view the results. Continuing support can be offered in addition to the original contract, thus providing the consultant with an additional source of revenue.
2) The consultant installs the software as in option 1, but provides no support/training beyond running the model to demonstrate that all files are present.
3) Agency staff receive, install, run, and verify the modelling files to ensure all files are present and the model runs to completion.
4) Model files are transferred to the agency on a permanent hard drive and permanently stored at the agency offices.
5) Model files are stored at the consultant's office for later retrieval when needed.

The first three options reproduce the documented model results and provide a conclusive test for complete transfer of the correct files. Experience has shown that the last two options, where files remain unchecked, often involve higher costs for future retrieval. Therefore, it is recommended that the last two delivery options be avoided.

Based on ORMGP experience, the best means of ensuring that all model files are properly delivered is to demonstrate that the model runs on a computer that is independent of the consultant's professional network (options 1 to 3). This will identify any missing or corrupt files and helps avoid future recovery costs. Option 1 is preferred over the others since installing and running modelling software often requires technical expertise as well as software specific experience, and the basic training will help to drastically reduce staff time related to future model use. The model delivery, and hence the project, should not be considered complete until all files have been successfully transferred to the client's specifications as outlined in the RFP/contract.

As a best management practice, it is recommended that the consultant transfer the originally provided data back to the client agency as part of the final project delivery. This is recommended even in cases where the data have not been altered by the consultant, since the database at the agency may have been updated during the course of the modelling study such that it no longer reflects the original data provided at the project start-up. This ensures that the data used for model development is readily available to anyone wanting to check or rerun the delivered model to perform post-audits.

It is important to remember that data storage is relatively cheap when compared to the cost of reproducing the model files or when compared to the cost of going back to the consultant after long periods of time to have them try to locate the needed files or recapture the model results. Agencies should never be deterred from accepting large quantities of data.

FINAL DELIVERY CHECKLIST

The United States Geological Survey (USGS) has a checklist of questions that must be addressed prior to a model being accepted (Martha Watt, personal communication, 2015), and serves as a good example to follow. The checklist, provided here, details data requirements that all agencies and consultants should consider when delivering model files.

- Are all of the files there to run the model?
- Are all of the files there to run each simulation documented in the report?
- Are there extra files? Delete extra files.
- Are any files empty? Delete empty files.
- Are the file names easily understood to the outsider?
- Is the structure of the directory holding this information easily understood?
- Is the data organised into input and output directories?
- Is the source code included with the model files?
- Can the model be run?
- Can the results be matched to the results documented in the report?
- What other data are available to check in tables and text?
- Can these data be verified by model input or output data?
- Are the figures, text, and model input and output all consistent?
- Is there a README file?
- Does the README file contain all of the necessary information?
- Is there an information file that contains the spatial boundaries and coordinates of the model?

5.7.2 Model Report

A standardised model report structure is helpful because it enhances comparability and simplifies information access and retrieval. The model report should only contain information relevant to the particular study. A standard scientific format that incorporates executive summary, introduction (project scope), methods/model development, results, discussion, and limitations is recommended. The following sections provide some direction as to what each report section should contain.

5.7.2.1 Executive Summary

There are many parties that may be interested in the modelling work, yet most will not have the technical background or the capacity to review the report in full. This section should be kept brief and provide an overview of the project scope as well as the high-level results and overall implications of the findings. This summary should be limited to 2–5 pages.

5.7.2.2 Introduction

The introduction should focus on the project scope with just enough background information to place the study into an agency or resource management context. Discussion on consultant experience and expertise should be avoided, as these details will likely be a repetition of the proposal.

5.7.2.3 Methods/Model Development

The methods/model development section will likely need to be subdivided since model development typically occurs in stages (i.e., fieldwork, data collection and synthesis, model conceptualisation, model formulation, calibration and validation, etc.). The section should include:

- a description of the processes, procedures, and assumptions made in developing the model;
- an outline of the conceptualisation of the modelled system (this should be well referenced, clearly identifying areas where conjecture was applied);
- documentation of all model evaluation approaches, tools, and techniques that were applied (if parameter estimation routines or uncertainty analysis was performed, then a full description of the methods used should be included);
- documentation of procedures required for running the model including a list of all the steps (from a methodological perspective) used to generate the results, a list of the software tools that were used, and the file naming convention used for the model delivery package.

5.7.2.4 Results

The results section should address the results of the modelling work with specific reference made to what was requested in the RFP, and what was agreed to in the consultant proposal.

5.7.2.5 Discussion

This will be the most important section from a model management and custodianship perspective, as it should detail the effectiveness of the model to address the agency's original problem, highlighting issues related to model uncertainty and the implications on water resources–related decision-making. In addition, this section will provide comment on the models' future applicability outside of the scope of the current project. If requested in the RFP, then this is an opportunity for the consultant to provide their vision as to how the model could be continually operated into the future. The following should be incorporated:

- detail the success of the model in addressing the issue at hand, noting any improvements on past modelling efforts and possible future uses;
- highlight how the model has provided new insights (or confirmed suspected ones) into the overall understanding of the environmental system;
- discuss any concerns encountered (e.g., technical limitations, data gaps, etc.) during model development and recommend means for improvement;
- discuss the uncertainties inherent in the model, listing the assumptions and expert judgements made by the modeller that may affect model performance and evaluation; also mention how the uncertainties have a bearing on the model results and on future use of the model; and
- suggest further model improvements as part of the agency's ongoing model management strategy.

5.7.2.6 Limitations

This section should provide cautions to the agency regarding the use of the model, its predictive capacity, and constraints to the model results, beyond which misinterpretation of model results could lead to erroneous decision-making. A clear description of the model's original scope/intent should be re-stated.

5.7.3 Tables and Figures

Tables, figures, and maps used within the report should also be submitted as separate files, such that they can be used for future reporting and presentations.

5.8 MODEL FILE MANAGEMENT AND DIRECTORY STRUCTURE

The United States Geological Survey's (USGS) New Jersey Water Science Centre has put forward a generalised model file directory structure (see inset box) that has been successfully used for archiving/maintaining models at the federal level and in New Jersey. Models are distributed to external parties on request, but no updates are re-incorporated; only USGS-built models are included in the management structure. If a model is significantly updated by a USGS researcher, then, rather than altering original files, a second model archive is established, which would reflect the updated research.

The directory structure that has been implemented at the ORMGP was influenced by the USGS README file components; however, instead of simply listing properties of the model, a directory-tree structure was created to satisfy the program's long-term model management program. This implemented directory structure was found to be highly effective for: i) maintaining a project overview; ii) providing an intuitive means of model file recovery; iii) allowing users/agencies/consultants to readily determine where to put new files; iv) capturing and storing model files in a standardised format; and v) allowing new staff or third parties to more easily understand and build on the original work. The directory structure is outlined below and is put forward as a recommended best management practice for widespread use in efforts to move towards a standardised approach for the province.

The recommended directory structure has been designed taking into consideration that numerical models will continue to be used into the future. As a result, it should be recognised that the agency and the consultant have a shared responsibility to jointly manage the proposed file structure as outlined below. It is important for the RFP to speak to the proposed file management layout at the start of any modelling project so that the consultant can establish the file directory structure right at the onset of the project.

USGS FILE DIRECTORY STRUCTURE

The United States Geological Survey (USGS) directory structure (Martha Watt, personal communication, 2015) includes the report, model source code and compiler, final calibration runs, scenario runs, sensitivity runs, and particle tracking. Overarching the model directory structure, the USGS includes a README file saved within the root directory of every model. The USGS README file requires the following information:

- Disclaimer
- Introduction
  - Report name, number, and series, and authors
  - Type and version of the model used (e.g., MF2000, MF2005, SHARP) and the FORTAN compiler used
  - Units modelled (distance and time)
- Input file installation
- Data description
  - Number of simulations
  - Directions for using name files for scenarios
  - List of different simulations with name file
- Replicating simulations
- GIS data
  - Projection information
  - The coordinates for all four corners of the model grid, the reference used (e.g., NAD83), and angle of rotation (if any)
- Replicating particle tracking (if it was done)
  - Number of runs
  - Particle tracking methodology (e.g., forward, backward)
  - List of all the response files and description of particle tracking
  - Endpoint and pathline files
- Parameter estimation and the code used
- List of all of the files with description
- References
- Name of README file created by the consultant or USGS researcher

The directory structure presented below (adjusted from the USGS version by the ORMGP) is designed to follow the progress of a typical modelling project. The first four directories are the responsibility of the agency commissioning the project, and are built either prior to or over the course of the modelling study. Directories 5 through 8 would be the responsibility of the consultant and their transfer to the client would essentially complete the model delivery at the end of the project. It is strongly recommended that this directory structure be specified as a requirement within the RFP. The final three directories (9–11) are required for the long-term utility of the constructed model(s) and are recommended in order to streamline the process of model delivery to future consultants who have been contracted to build on the original model. It will also help facilitate the internal use of the model by the agency. Only these last three directories are expected to be modified over time.

1. Start-Up

- This directory contains all documents that describe the modelling study context: the RFP, submitted proposals, any agency partnership agreements, terms of reference, contracts, etc.

- Agencies should consider retaining the proposals from all bidders (not just the successful consultant) for reference in future projects.
- This directory is assembled by the client agency.

2. Original Data

- This directory will hold the data delivered to the consultant at start-up. This preserved copy will serve as a reference if there is a question as to what data were available and provided to the consultants.
- This directory is assembled by the client agency.

3. Related Projects

- In cases where a model is an extension of a previous model(s), or a refinement of an existing model(s), this directory will serve to preserve those linkages at the time of delivery.
- This directory could also contain links to related project reports, if documents are managed within a digital database.
- Reports provided to the consultant for earlier conceptualisation exercises for the purposes of model construction will be contained here.
- If additional reports are discovered by the consultant during model conceptualisation, they can be stored here as well.
- It is recommended that a subdirectory structure be used to separate sources (e.g., scientific literature, previous technical studies, fact sheets, etc.).
- This directory is first assembled by the client agency, but both sides can make additional contributions during model development.

4. Communications

- This directory will contain documentation that logs progress as the model is developed and will include such documents as work logs, meeting minutes, interim presentations, review comments, draft reports, emails, etc.
- This directory will be assembled by the client agency with contributions from the consultant.

5. Model Delivery

- Model files provided by the consultant at the end of the modelling project will be stored in their original delivered format. It is recommended that they never be altered (i.e., any updates or changes made by the client would be made on a second independent copy of these files, which would be held in the Operational Model directory – see below). This will preserve files for the sake of record keeping and versioning.
- This directory contains all the data required to run the model and replicate the data contained in the Model Outputs directory.
- Subdirectories could include:
    - model input files (structural, control, parameter, variables);
    - spatial data and relational lookup tables;
    - corrected data (i.e., start-up data that has been corrected, infilled, interpolated, etc.);
    - calibration/validation/baseline model;

  - model scenario(s) – one scenario per subdirectory;
  - model uncertainty/sensitivity analysis;
  - particle tracks, drawdowns;
  - other model runs (i.e., steady state, coarse resolution, regional model used to determine boundary conditions, etc.).
- This directory to be delivered by the consultant at the end of the project.

6. **Model Outputs**
   - Original direct model outputs – again it is recommended that this directory never be altered so files will be preserved for record keeping and versioning.
   - This directory is likely to become quite large and may require selective archiving, compressing, or simply be stored elsewhere. Everything contained should be reproducible using the files stored in the Model Delivery directory. For agencies with greater technical capacity to rerun the models, this directory can possibly be deemed redundant; this is the main rational for separating model outputs from the model delivery (two independent directories).
   - This directory to be delivered by the consultant at the end of the project.

7. **Model Executables**
   - This directory will preserve model code used in the study recognising that future updated versions of a code might not work with the format of the delivered model files or where a source code is discontinued from widespread use and therefore difficult to acquire or find in the future.
   - A subdirectory should be created if there were any scripts and/or model code modifications made. The subdirectory would be provided by the consultant and would contain either the original script(s)/code modification(s) or a detailed description required for reproducibility and future reference.
   - This directory should also contain details of all associated software and versions used for the modelling in the form of a README file (e.g., the modelling software, data analysis software, post processing and visualisation software).
   - This directory to be delivered by the consultant at the end of the project.

8. **Model Report**
   - Official final report will be held here.
   - A subdirectory should be created here that contains model-derived results including spatial data and tables used as part of model report development, such as:
     - model results (extracted from output files either by hand or using post processing software tools);
     - GIS files;
     - parameter tables; and
     - databases.
   - Data should be provided in a consistent/standard file format as described above.
   - This directory to be delivered by the consultant at the end of the project.

9. Miscellaneous

- A supplemental area for additional information unique to each particular project.
- Provides flexibility to store information that does not easily fit elsewhere.
- The directory could theoretically acquire additional files well after the completion of the project and delivery of the model.
- This directory is to be established by the client agency with contributions from the consultant as needed.

10. Operational Model

- This directory will either contain an active version of the model or will provide a pathway/link to where the current/operational version of the model is located on the agency server/workstation.
- Initially, this directory would be identical to the Model Delivery directory, but here files are allowed to be modified. Preserving the model in its delivered state elsewhere, allows for the model to be tested and rerun without worry of mistakes since they can simply be alleviated by resetting the model to its original state.
- The model could be used for internal agency purposes.
- If needed, the model files could be efficiently packaged in a subdirectory so that they could be readily transferred to future users.
- This directory would be created by the client agency and would be actively managed by the model custodian.

11. Future Use

- Should this model be updated at a later date, a new directory structure will be built to document the new project. Within this directory, a link to the new model directory will be added for later reference and version control.
- This directory would be managed by the model custodian.

5.9 MODEL FILE SHARING

Public sector agencies are currently receiving requests for complete modelling packages from consultants who are working for private clients. Public sector agencies, however, are struggling with how to address such requests given a host of concerns. Of particular significance is the misuse or misinterpretation of model results by a consultant to make an incorrect interpretation. Public sector agencies are concerned that models may be altered and used against the agency, such as at a hearing. In such instances it can take enormous resources, in terms of money and/or technical staff time, to investigate as to how models have been altered to arrive at differing results. The legal and governance challenges with respect to model file sharing have been discussed in Section 4. As for considering model sharing within a model custodianship program, challenges relate to how and in what form the model files are to be delivered.

The ORMGP is looking to develop an online data portal that would include a Model File Request form containing a brief questionnaire that needs to be filled out in order to gain access to modelling files. The questionnaire is envisioned to ask relatively simple and straightforward questions such as:

- Who is requesting the data (individual, public sector agency, consulting firm)?
- What project would the model(s) be applied to (provide a brief description)?
- Is there an intention to modify the model? If so, will the party agree to return (if requested) any changes in digital format, as part of a model sharing agreement?

Posted with the questionnaire, would be a disclaimer that would transfer all liability from the model owner to the requesting party such that they would assume all responsibility for the outcome of their work with the model. The disclaimer would also specify that all costs associated with clarifying anything related to the model files, or to the use of the model itself, would be borne by the requesting party. The disclaimer agreement would need to be signed before modelling files would be released. A sample disclaimer, similar to what would be posted, is provided in Appendix 3.

Upon receipt of a signed disclaimer, a decision would be needed as to what exactly would be released as part of the model transfer. There are many degrees of data/file transfer that can be proposed, and it is recommended that this decision be made by a model management team, which would include the model custodian as well as technical staff from the agency who owns the model.

In response to a request by a third party for a numerical model, there are several responses that can be put forward by the public sector agency. These include:

1) Refusal to share any of the model files.
   This approach would likely be unsatisfactory to the third party, as well as to senior management at the public sector agency since it is contrary to the spirit of fostering cooperation and would lead to allegations of agencies being secretive with files that were paid for by public funds. The only time that this could prove to be a justifiable response would be if the model was outdated or was deemed to not reasonably reflect natural conditions in the field. A documented justification of such a condition should be readily available with the files associated with the numerical model.

2) Open access to all models and associated files so that they can be used by third parties for their purposes.
   This type of sharing is ideal in that it fosters increased expertise within the consulting community since, in theory, there would be an advantage to those consultants who could make use of numerical models. This complete transfer would be the ideal situation for the consultant and their client since they would be able to make use of the data and/or the model for their purposes. Although it would be difficult to administer, public sector agencies would likely want to ensure that the model (or any of its components) would be used only for the active project for which the consultant is working upon. A model sharing agreement could be signed, which would limit the use of the model (or any of its components), so that agencies know where and how the model, and/or any component of the model (e.g., data, surfaces, etc.), is being applied.

Examples of data/model file sharing agreements, which can be used in whole or in part, are found in Appendix 3. In addition to the data sharing agreement, certainly each agency would want to ensure that a disclaimer (see Appendix 3 for an example) is also transferred with the model files such that any responsibility for the use of the model rests with the model user.

3) Delivery of the model files similar to above, however, only data relevant to the described model request would be provided with the signing of a data sharing agreement.
   This case is the same as above except for the treatment of the database that is a key input to the model. In addition to concerns about inappropriate use of the model, if the model is regional in scope then data that is outside of an agency's jurisdiction could be transferred to a consultant unbeknownst to the adjacent agency. Agency staff might be reluctant to release a data set, especially in cases where it extends outside of their jurisdiction. In such cases it might be advisable to separate the database from the model and handle transfers to outside parties with separate agreements and disclaimers. Even in cases where the database is not transferred, this should not prevent the rerunning and use of the model by an outside party.

4) Delivery of the model essentials or building blocks (e.g., geological layers, geospatial data, land use, bathymetry, climate data, hydraulic conductivities, etc.) such that the consultant can use the provided data to build a new model in the vicinity of their project area.
   In cases where a public sector agency might be uncomfortable with the transfer of an entire built numerical model for the use of outside parties (for whatever reason), it is still possible to maintain an open transparent transfer of model components. With the transfer of essential model elements, the consultant could rebuild a model without the large expense of reinterpreting data and re-encapsulating, in digital format, the established conceptual model for an area. This approach still facilitates knowledge exchange and advancement of the model, however, it might minimise the misuse of the model since in this case there is additional burden on the consultant to think through the model reconstruction and the assumptions that were built into the original model. An improved model might result. It is still recommended that model sharing agreements and disclaimers also accompany such modular transfer of numerical model components

A follow-up topic related to model file sharing is the question of determining which model an agency might release to a consultant, especially in geographical areas where two or more overlapping models exist. In cases of two overlapping models, it may prove in some cases that the conceptualisation from model A is preferred over model B, however, aspects of the parameterisation from the model B is preferred. Such cases demonstrate the need for managers to be nimble in understanding and managing their numerical models and the components or building blocks from which they are built.

Agencies are encouraged to ensure that a custodianship program is put in place to help review and determine which model best reflects the physical reality of the flow system and that their model file sharing procedures take into account this concern. Again a number of options can be taken by agencies looking to manage and share numerical models:

1) allow the consultant to select the model which best meets their needs;
2) allow the consultant to pick and choose components (building blocks) from any of the available numerical models;
3) provide to the consultant the most acceptable model (as recommended by the model custodian); or
4) provide the agency's authoritative model, which ideally would be deemed the model most trusted and accurate by technical staff for assisting in the decision-making process (ideally, this model would have been built and managed such that it incorporates the best and up-to-date interpretive components from all previously built numerical models).

It must be kept in mind that a consultant's model-based decisions and/or recommendations (using a shared numerical model) may well come back to the agency (or a partnered agency) for approval. For example, to evaluate a proposed development application, a consultant may use a shared numerical model to determine that any impacts would be negligible, and then prepare a technical report in support of an Official Plan Amendment (OPA). It is therefore important that prior to the sharing of numerical models/files that agency staff give due consideration to model sharing.

6 SUMMARY

Given the finances that have been invested in Ontario's source water protection (SWP) numerical modelling efforts, it is now incumbent upon water resources managers to ensure that the models are maintained and used into the future as tools to aide in the management of Ontario's water resources. The use of numerical computer models to assist in water management–related decisions should now be considered essential in Ontario. Successful numerical modelling studies require the collaborative work of public sector agency staff and technical consultants. This document has provided an overview of the key technical (Sections 2 and 3), legal (Section 4), and administrative (Section 5) considerations that should be incorporated into successful numerical modelling water resources management studies.

6.1 KEY MESSAGES

The cyclic nature of policy making implies that numerical modelling, upon which policies are based, is not a one-time effort. Rather, in an iterative manner, numerical models and related assessments should be regularly improved and refined. The management of model-derived knowledge over long time horizons, in explicit consideration of the three cycles discussed in Section 3, has many implications for how the modelling process should be best managed. In summary, key messages for model managers include:

- Weigh policy objectives against modelling resource needs.

  When designing and planning a modelling study, the total (i.e., short and long term) modelling resource needs should be balanced against the overall policy objective. For example, consider the case where a well might be situated in a highly complex terrain with complicated flow systems. Rather than embarking on a costly, long-term modelling study, it might be that a simple, readily implementable risk prevention option is available (e.g., move the well). This may prove more practical and more cost-effective than a long-term path of repeated model refinement. The long-term considerations of how a model might be used for other management issues must also be part of this evaluation.

- Broadly assess the longer term opportunities that modelling may provide.

  In considering the iterative process of policy design, implementation, and adjustment, the opportunity to refine an existing numerical model may arise when new technology or differing perspectives from other disciplines become available. This situation, where an existing model (or a newly proposed model) may be used to provide input into achieving several different policy objectives, should be anticipated and may warrant an early scoping study to identify future opportunities or potential issues that may be addressed with the model under consideration.

- Ensure model results are reproducible.

  This is an important principle for science-based decision support and defencibility. A numerical model reflects expert opinion that coherently integrates measurement data with science into a computational framework. In a complex world with limited available data, experts can often explain an observed phenomenon in multiple ways by applying different scientific laws (Beven, 2001). Model results reflect the opinion of one individual modeller or a modelling team. It is important to keep in mind that water management decisions that are based upon numerical model results can be challenged. Therefore, the model results must be reproducible such that agency positions can be defended, corroborated, refined, updated, or adjusted if needed.

- Consider partnerships for modelling studies.

  Where multiple agencies are implementing similar modelling processes, there are likely great benefits to coordination, standardisation, and shared tools. Standardising across more than one agency (e.g., in terms of data management, modelling processes, formats, and/or the common use of software/licencing) will reduce costs and generally increase the transferability of modelling products, alleviating issues related to reproducibility. Partnering in areas related to modelling infrastructure allows for the sharing of information technology investments and for the effective exchange of knowledge, services, tools, documentation, guidelines, training materials, and staff.

- Several factors need consideration in the conceptual and technical cycles.

  From a management and budgetary point of view, the challenge of these two cycles is to create a balance amongst: i) low overall cost; ii) quick turnaround within the overall timeline of the larger policy cycle; iii) sufficient quality to maximise the effectiveness of model-supported water management decisions; and iv) longer term maintenance of relevant water resources knowledge, which can be generated for future uses of the model.

- Consider model complexity.

  Highly complex and detailed models may require less incremental improvement and adjustment, but have very high initial costs. On the other hand, simplistic models have low initial costs, but could require more costly follow-up cycles of data collection and model refinement requiring repeated access to external experts. Simplistic models tend to be limited in scope and may not be useful for broader application without significant revisions.

- Avoid costly modelling for simple situations.

  In many cases, model expectations are inconsistent with data availability and system knowledge. In cases of limited data and knowledge, models can only deliver very limited insight and the public may be better served by using traditional non-modelling approaches, such as field monitoring programs. In other cases, modelling costs can be reduced dramatically using common sense. For example, it is not necessary to set-up complex models in order to demonstrate that a very large contaminant source located in the immediate vicinity of a surface water intake may pose a risk of contamination (Arnold, 2013). Complex models are best suited to determine risk levels in situations where sufficient observation data exists and system behavior is not intuitive. This situation requires intensive learning from study participants.

- Plan ahead for modelling knowledge needs.

  Modelling is inherently knowledge intensive requiring location-specific, scientific, procedural, engineering, programming, and managerial knowledge and skills. The data required for most modelling studies can be anticipated and thus should be collected and processed prior to retaining a modelling consultant. The modelling process can also benefit greatly by effectively implementing knowledge management workflows (e.g., by using commonly known/standard software packages, avoiding self-tailored software routines, ensuring adequate documentation standards, using common databases and file formats, using shared terminology, establishing support mechanisms across agencies, etc.).

- Consider investment in automation and integrated modelling frameworks.

  Given the cyclic nature of modelling, model refinements are to be expected. Therefore, initial up-front investment in software-based automation may help reduce the cost of each conceptual and technical refinement cycle. Tools can be developed as stand-alone executables, or within a graphical user interface. Alternatively, integrated modelling platforms will continue to exist that can coherently store data, facilitate scenario design, transform data into input files that are readable by several model codes, and offer tools for processing, analysis, and visualisation of model outputs. They can also help to ensure the reproducibility of results.

- Consider access to modelling codes and intellectual property rights.

  Modelling codes and related software tools are used to run the model and for related processes, such as the cleaning of raw data, the creation of model inputs, the analysis of model outputs, and the visualisation of results. Without access to these tools, models cannot be rerun or updated, nor can the results be reproduced. In a cyclic/iterative modelling paradigm, long-term access to these products is paramount. The following points should be considered when selecting a model code or any software tools, whether they are created through private companies, universities, or government research groups: i) future code longevity (e.g., company track record, financial viability, financial stability of government or university research teams, etc.); ii) history of code maintenance and upgrades; iii) longer term affordable access; and iv) support services.

- Consider standardisation.

  Standardisation can take many forms and can apply to many aspects of modelling such as: i) processes; ii) software design; iii) data formats; iv) data transfer; v) data processing routines; vi) visualisation rules and templates; vii) modelling frameworks; or viii) prescribing modelling software. Although agencies and consultants frequently prefer to maintain flexibility in many of these modelling aspects, at the same time, standardisation may greatly reduce modelling costs.

6.2 A WORD ON FINANCES

Given that this document proposes that numerical models be carried forward for future use, it may prove helpful to provide a comment on ways and means to finance ongoing or future model-related activities (e.g., database/model updates, management, and maintenance). Initial development of the numerical models for the SWP program was largely paid for through provincial funds that were allocated to municipalities and/or conservation authorities. However, in moving forward, it doesn't appear likely that the Province will be providing future model-related funding.

As an initial priority in minimising future modelling costs, agencies should give due consideration to partnering with adjacent agencies to distribute costs. Again, drawing on the Oak Ridges Moraine Groundwater Program as an example, here the ongoing costs for data and numerical model management have been distributed across partner agencies such that the financial burden on any one agency is manageable. Although the costs to cover model management–related activities could come from general revenues, other options can also be considered, including:

1) **Fee for model use** – rather than making the models available for others to use at no cost, agencies could consider charging a fee to make use of an existing numerical model. The fees collected would then be directed to maintain/update the model. Such a fee could differ depending upon whether:
    - the consultant only makes use of model components (e.g., database, spatial data, monitoring data, geological layering, etc.);
    - the consultant runs the model themselves;
    - they request that the agency run the model for them (provided expertise is available); or
    - the agency oversees the running of the model through a different consulting firm.

    A concern with this approach is that consulting firms may be unwilling to participate and instead may propose to their clients that a new model might be a better approach. The resulting funds thus attained for model management might be limited.
2) **Model/data levee** – currently many municipalities and conservation authorities have a fee structure in place for reviewing development applications or for commenting on environmental assessment reports. Given that these types of studies could benefit from the use of models, an argument could be made that an additional general environmental data/model management fee be imposed on top of the regular fee that is charged to developers.
3) **Water rate charge** – in cases involving municipalities that oversee water distribution systems, a water-related data/model management fee could be added to water bills with the collected funds being allocated strictly to data/model management activities.

In addition, there are likely other funding avenues that could also be pursued. However, it could also be argued that the pathway of rigorous data management coupled with numerical modelling has become such an important approach to model management that it should be funded as part of regular every day work.

NUMERICAL MODEL COSTING

Certainly numerical modelling is recognised by most public sector agencies as a costly endeavour. However, for many agencies the costs can still be an unknown factor when trying to determine a future water resources management pathway. The final cost for watershed modelling is of course dependent on many variables and it is difficult to approximate what a numerical modelling study might cost. The discussion here provides an idea of the costs associated with numerical modelling as well as identifying factors that can assist in holding down modelling costs.

As a benchmark, the Ontario Ministry of Natural Resources (MNR) reported that between roughly 2007 and 2014 Ontario-wide source water protection (SWP) water budget–related costs amounted to some $27 million. These costs were tied to activities related to the water budgeting component of the SWP, much of which was directed towards numerical modelling. On a case by case basis, SWP modelling studies ranged from on the order of $50K to $100K for smaller tier 2 studies where data accessibility was not a significant issue, to on the order of $1.5 million for more complex integrated tier 3 models. Modelling consultants typically charge their time out at rates of $100/hr to $200/hr, depending on the experience of the modeller.

One of the most significant factors that can easily increase the costs for modelling is poor data management practices. Once consultants are given the go ahead to begin a modelling study, it is critical that the public sector data has been reviewed, properly organised, any errors or omissions addressed, and that it is readily available for transfer to the consulting team. Considerable costs can be accrued by modelling consultants as they try to use poor quality data to begin the model building process. Going back and forth with data checking and missing data are not only costly in terms of finances, but it also delays the project, and sets up an unnecessary tension between the client and consultant.

Another factor that can drive up modelling costs is when the question to be answered is not clearly asked. Experience has shown that modellers can create either too simplistic a model for the client’s purposes or too complex a model. Even just exploring incidental processes that are not relevant to the issue at hand can prove costly. As an example, consider a public sector agency that asks a modelling consultant to determine the flow dynamics of a river at a particular road crossing. The consultant may deliver a model that provides an estimate of flows in the river. However, in review, the client then makes it known that they are more interested in the pathways that water may take to arrive in the river (which might answer a question such as how would land use change affect the timing of water arriving at the river). Once this is revealed, the model may need to be re-opened, incurring additional, unbudgeted costs. It is encouraged that the RFP fully focus on the issue to be resolved and clearly state the question that needs to be answered. This will reduce the chances that a delivered model will be unsatisfactory.

In moving forward, given the situation in Ontario, where there may be more than one available model that covers a specific area, it may prove costly to request that the modelling consultant determine the best available model for any particular project. This would require that all models be opened up and researched to see which one provides the best fit for the project at hand. A preferable, and more cost-effective, option would be for a model custodian to have already run and reviewed the models and to provide immediate direction as to which model is the most appropriate.

6.3 Considering Agency Roles in Numerical Modelling

To date, there has been little guidance put forward in the province for the continuation of numerical modelling in terms of the roles agencies should play in facilitating the future use, maintenance, and improvement of numerical models. There are constructive roles for all agencies in moving ahead with model management. Certainly in terms of data collection and management, a key component of numerical modelling, all agencies have a role to play in developing sound strategies. Ideally, databases should be openly accessible and cooperatively managed amongst agencies, ensuring transferability of data between agencies and establishing means for staff to build upon earlier collected information.

In terms of fostering the ongoing and future use of numerical models, again all agencies have important roles. At the provincial level, the role may be as straightforward as requiring the use of numerical modelling in various policy initiatives. Municipalities and conservation authorities can request from consultants and other practitioners that existing models be used to assist in providing critical input to strategic water resources management decisions. Policies can be put in place at either the provincial or municipal level that require the updating of numerical models to support water resources decisions.

When making water resources–related decisions, technical staff from all agencies, at the federal, provincial, and municipal/conservation authority levels, have the responsibility to become familiar with available models and the key insights into the hydrological system provided by the models. Providing input into or making water resources–related decisions without taking the time to review and integrate numerical model insights will lead to weak and unsatisfying water resources decisions for Ontarians.

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APPENDIX 1

GLOSSARY OF MODELLING TERMS

Boundary condition — a mathematical expression of the state of the study system, which constrains the equations of the mathematical model. In a physical system, boundary conditions define the flux of material and energy across the spatial boundaries of the study system (e.g., groundwater recharge, lake stage). An example of a boundary condition would be a no-flow boundary, for example, at a watershed divide where no surface water (and maybe also no groundwater) would cross.

Calibration — procedure of adjustment of model parameters needed to reproduce observed (i.e., measured) phenomena within the range of accuracy specified by a set of performance criteria (Beven, 2009).

Cleaned or corrected data — raw data that have been reviewed and screened for measurement or systematic errors and data gaps. The errors are removed, adjusted, or simply flagged as being suspect; data gaps are either infilled or flagged as missing.

Conceptual model — description of reality in terms of verbal descriptions, equations, governing relationships, or natural laws that purport to describe reality (Refsgaard et al., 2005), or an interpretation or working description of the characteristics and dynamics of the physical system (ASTM, 2016).

Confirmation — determination of the adequacy of the conceptual model to provide an acceptable level of agreement for the domain of intended application, such as model scenarios (Refsgaard et al., 2005).

Cyber infrastructure — integrated system for automated collection, storage, retrieval, and analysis of data that are accessible by multiple parties. Tools support real-time collaboration with other remotely based researchers and provide access to the monitoring information collected by an observatory's field facilities, as well as historical and other relevant data. Analytical, statistical, modelling, and visualisation tools needed to conduct engineering analyses are provided within the system. An operational cyber infrastructure could also include control and feedback systems for decision-making and management (Driscoll and Reible, 2007).

Ensemble modelling — process of utilising multiple models and formulating the results as a single score with a given uncertainty. The ensemble modelling approach improves the certainty and thus confidence in the predictive capacity of the numerical analysis. Multi-model ensembles can be generated by varying the parameters of a single model structure, varying structural elements of a single model code, or by applying several different model codes to the same study area.

Forcings — set of model input data that stresses the numerical model for the purpose of observing a model response. For example, an extreme rainfall event (forcing) causing a flood (response).

Global sensitivity analysis — sensitivity analysis methods that vary multiple input parameters over the full parameter space in order to explore the impact of parameter uncertainty on model outcomes (Saltelli et al., 2008). Global sensitivity analysis generally has three steps: i) selection of representative parameters; ii) multiple model runs with input files representative of (selected) parameter space; and iii) systematic evaluation of the relationship of model inputs to model outputs (see also 'sensitivity analysis').

Input files — data files that are read by model code. Input formats are generally specific to a particular model code. Input files are formatted from corrected data by changing spatiotemporal resolution and/or by infilling data gaps by interpolation.

Integrated model (in hydrology) — models that simultaneously simulate a combined set of hydrological processes. Integrated models simulate the processes involved in groundwater, surface water, and overland flow in a watershed.

Local sensitivity analysis — sensitivity analyses methods that are based on a particular parameter value. The method varies a single parameter while keeping all other parameters constant (Saltelli et al., 2000), and observing how sensitive the model results are to the changes in the particular parameter. Local sensitivity analysis assumes parameter independence and a linear relationship with model results, which is often not the case with environmental models (see also 'sensitivity analysis').

Model — working analogy of a real object (or system). Modelling provides the possibility to simulate and predict the behaviour of a real object (system). Due to the model's incomplete representation of the real object, a model may give a distorted view of certain aspects of the real object that may lead to false conclusions (Hattermann et al., 2010).

Model-based scientific policy advice — recommendations that have the objective to influence policies and that are derived from numerical modelling.

Model code — generic software program that can be used to address different problems in different study areas without modification to the source code (Refsgaard et al., 2010). The model code assembles the numerical model, data management and accounting, and the control language used to define: i) a chosen model structure, ii) model parameters, iii) location and form of input data, and iv) types and form of output data (ASTM, 2016).

Model evaluation — process of determining model usefulness and estimating the likelihood of relevant outcomes. Model evaluation methods typically involve the creation of a number of input files following an experimental design (e.g., scenarios) and the subsequent generation of many output files. From a systematic evaluation of these outputs, an understanding of model behaviour and the uncertainty of model results is determined. This constitutes the model evaluation.

Model realisation — solution given by a numerical model from a unique set of input parameters. As there is inherent irreducible uncertainty in model input parameters, there will consequently always exist a number of unique model realisations/solutions that are all equally plausible given data availability.

Model response surface — given a set of model realisations, the response surface reflects the models ability to reproduce observations from a given set of input parameters sampled from the parameter space.

Model results — information generated through the use of a model code. Model results are extracted from output files either by hand or using post-processing software tools. Model results are interpretable by non-experts and are generally easily communicated.

Model set-up — establishment of a site-specific model using a model code, a conceptual model, knowledge, and observations. This requires, among other things, the definition of boundary and initial conditions and parameter assessments from field and laboratory data (modified from Refsgaard et al., 2005).

Model structure — describes how the most significant and dominant flow mechanisms and processes are represented within a model code (Butts et al., 2004). Typically, during the conceptualisation phase, the model structure becomes fixed and calibration is obtained through the adjustment of model parameters.

Model uncertainty — uncertainty associated with numerical models. All models bear inherent uncertainty, which will limit the confidence in model results and hence in any model-related decisions (Refsgaard and Henriksen, 2004). Model uncertainty can be tied to the following: i) the incomplete knowledge of the conceptualisation of the system being modelled, model parameters, input files, and/or boundary conditions; and ii) the simplified description of the real world into the numerical model. Uncertainty can be characterised (Walker et al., 2003) by its:

- sources: model conceptualisation, model structure, boundary conditions, input data, parameter values, technical errors; uncertainty in model results will propagate given the combined effect of these errors;
- nature: epistemic (imperfect knowledge); aleatory (stochastic/inherent variability).

Numerical model — set of mathematical formulations that follow a certain logical procedure to describe physical system behaviour given certain simplifying assumptions (ASTM, 2016) and calibrated parameter values (Refsgaard et al., 2005).

Output files — files written after running a model code. Output files are characterised by the variables that are saved (e.g., hydraulic head, streamflow, etc.), the temporal and spatial extent and resolution of these variables, and the file format. In their original format as produced from the model, output files are generally not readily interpretable by non-experts and thus require post-processing to create model results.

Overland flow/hydrological/watershed model — numerical model purposed for water budget analysis involving interception, evapotranspiration, infiltration, runoff generation, soil moisture storage, and groundwater recharge. These models are often termed surface water models, a term which should be reserved for models that simulate hydraulics as opposed to hydrological processes.

Parameter space — multi-dimensional space that expresses the feasible range of model parameters. The number of dimensions equals the number of adjusted model parameters. Any point within parameter space represents a feasible model parameter set and would provide for a unique model solution. The combination of a point in parameter space and its unique model solution is often termed a model realisation.

Parameter uncertainty — uncertainty associated with the value of a certain model input parameter.

Performance criteria — level of acceptable agreement between model and reality. Performance criteria can apply both to model calibration and to uncertainty analysis (Refsgaard et al., 2005).

Quality assurance (QA) — procedural and operational framework, used by an organisation managing data and models, that assures: i) a scientifically adequate execution of all modelling tasks; and ii) that all steps of modelling workflow are reproducible and technically justifiable (National Research Council, 1990; Refsgaard et al., 2005; after Scholten et al., 2007[1]; Vanrolleghem, 2010, p.17).

Raw data — data, as measured or obtained in the field, either from: i) automated instrumentation (e.g., data loggers); or ii) from manual field observations. Raw data may contain measurement or systematic errors and data gaps.

Scenario — typically a hypothetical forcing or structure imposed on a numerical model for the sake of predicting potential impacts to the study system. In practice, model scenarios are used to describe: i) explicit human interventions (e.g., a contaminant spill, a pumping from certain wells/intakes, changes to the physical infrastructure, land use change, policy options, etc.); or ii) external global patterns (e.g., extreme events, droughts, climate change, volcanic eruptions, etc.).

Scientific gateways — web-based interface to access high performance computers and storage systems. Gateways allow science teams to access data, perform shared computations, and generally interact over the web.

Sensitivity analysis — methods of addressing a numerical model's relationship to: i) model parameters; ii) boundary conditions; and/or iii) input data. Sensitivity analysis is the study of how the uncertainty in the model output can be apportioned to specific sources of uncertainty in model structure or inputs (Saltelli et al., 2000). Sensitivity analysis covers a variety of strategies that quantitatively partition the model uncertainty into particular components (Refsgaard et al., 2005).

Study system — real, natural, physical system, understood here as a study area that is confined by spatial boundaries (Refsgaard et al., 2005).

Surface water model — application of a numerical model to represent surface water systems (waterbodies [e.g., lakes, wetlands, ephemeral pools] and watercourses [e.g., streams, rivers, canals, etc.]). The term surface water model is often used ambiguously to represent overland flow or

[1] This modification of the older National Research Council (1990) definition includes the organisational, technical, and scientific aspects, but in addition the need to build consensus among the organisations concerned.

hydrological models, however, technically, a surface water model should be relegated to those that model the physical movement of water (i.e., hydraulics).

Uncertainty — stems from the lack of confidence about the specific outcomes of an event or action. Reasons for this lack of confidence might include a judgement that the information is incomplete, blurred, inaccurate, or potentially false. Alternatively, the lack of confidence might reflect intrinsic limits to the deterministic predictability of complex systems or of stochastic processes (Refsgaard et al., 2010). Uncertainty also arises in situations where there is not a complete, unique, and objective understanding of the problem to be modelled (Brugnach et al., 2008).

Uncertainty analysis — describes a range of quantitative and qualitative methods to describe and communicate model uncertainty. The analysis takes into account the combined effects of all model uncertainties, such that their importance for the model results can be communicated (Hattermann et al., 2010).

Validation — process of substantiating whether model results have a satisfactory range of accuracy that is consistent with the model's intended application (Scholten et al., 2007). Model validation is usually performed using independent data that is not used for calibration (after Klemes, 1986). In practice, validation is often not feasible, there are philosophical limitations (e.g., Oreskes et al., 1994) and practical problems, that is, once a validation test has failed and a conceptual error is corrected, then there will be no more independent data available for validation, and calibration and validation become indistinguishable.

Verification — process that ensures no technical mistakes were made. Authors distinguish between:

- code verification — software testing, mass balance closure, comparison to analytical solutions, and comparison with other similar codes to demonstrate that the code represents its mathematical foundation (ASTM, 2016). Verification ensures that the model code accurately solves the equations that constitute the mathematical formulation (Refsgaard et al., 2005).
- model verification — determines that no technical mistakes were made along the modelling workflow, including software development (see code verification), model set-up, and interpretation of output files. Technical mistakes could include, for example, errors in data storage, data transformation, design of model, and output file processing. Verification must be performed by the signatories to the model study documentation.

Workflow — overall process of generating results from data with the use of a numerical model. If either the data or the model is updated, then all steps of the modelling workflow need to be repeated. Leonard and Duffy (2016) distinguish four types of workflows: i) data workflows that read and aggregate essential data sets used to construct numerical models; ii) data-model workflows that transform the data into model inputs; iii) model workflows that handle the distribution of data within the computational environment; and iv) visualisation workflows that create and share numerical model results for analysis and peer review. Workflow management continues to be one of the grand challenges of environmental modelling (Beck, 1987; Doherty, 2010), even though software is emerging that offers user interfaces for setting up workflows. Many consulting firms have invested in automated workflow infrastructure in order to expedite the model development process by avoiding the repetitive and intensive manual data assimilation steps.

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Scholten, H., A. Kassahun, J.C. Refsgaard, T. Kargas, C. Gavardinas, and A.J. Beulens, 2007: A methodology to support multidisciplinary model-based water management; Environmental Modelling & Software, v.22, no.5, p.743–759.

Vanrolleghem, P.A. (ed.), 2010: Modelling Aspects of Water Framework Directive Implementation, Volume 1; IWA Publishing, London, United Kingdom.

Walker, W.E., P. Harremoës, J. Rotmans, J.P. van der Sluijs, M.B.A. van Asselt, P. Janssen, and M.P. Krayer von Krauss, 2003: Defining uncertainty: a conceptual basis for uncertainty management in model-based decision support; Integrated Assessment, v.4, issue 1, p.5–17.

APPENDIX 2

ANNOTATED BIBLIOGRAPHY

1 GOOD MODELLING PRACTICES AND WATER

Good modelling practices have been or are being developed in multiple subfields within the diverse landscape of hydrological research and practice. This appendix provides a short overview (including abstracts and sometimes summaries or comments from the author) of publications considered most pertinent to discussions found in this manual.

The following sections are found in this appendix:

1) The detailed guidelines provided by ASTM for groundwater applications. This subdiscipline has long been performed by consulting industry in the regulated context of environmental assessments.
2) Guidelines on good modelling practices for hydrological modelling from academic publications and grey literature, separated into subsections on general hydrology, rainfall-runoff modelling, flood forecasting and watershed modelling, water quality modelling, urban water cycle systems, and groundwater–surface water interactions.
3) Guidelines on integrated environmental modelling from literature that deals with conceptual and technical challenges in multidisciplinary research projects.
4) Selected articles from other fields of modelling and software design, which have general appeal and relevance for model management.

1.1 ASTM Good Modelling Practices for Groundwater Applications

ASTM International, known until 2001 as the American Society for Testing and Materials (ASTM), is an international standards organization that develops and publishes voluntary consensus technical standards for a wide range of materials, products, systems, and services.

Groundwater modelling is a standard procedure within environmental assessments, these being required for many regulated application procedures. ASTM has developed and administers a range of guides for groundwater modelling:

ASTM D5447 - 04(2010)	Standard Guide for Application of a Groundwater Flow Model to a Site-Specific Problem
ASTM E1689 - 95(2014)	Standard Guide for Developing Conceptual Site Models for Contaminated Sites
ASTM D6025 - 96(2008)	Standard Guide for Developing and Evaluating Groundwater Modeling Codes
ASTM D6170 - 97(2010)	Standard Guide for Selecting a Groundwater Modeling Code

ASTM D5610 - 94(2014)	Standard Guide for Defining Initial Conditions in Groundwater Flow Modeling
ASTM D5609 - 94(2016)	Standard Guide for Defining Boundary Conditions in Groundwater Flow Modeling
ASTM D5611 - 94(2016)	Standard Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application
ASTM D5490 - 93(2014)e1	Standard Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information
ASTM D5718 - 13	Standard Guide for Documenting a Groundwater Flow Model Application

These guidelines reference the full modelling cycle, including aspects of the conceptual cycle as well as the technical cycle.

ASTM D5447 - 04(2010), Standard Guide for Application of a Groundwater Flow Model to a Site-Specific Problem

Summary:

Groundwater models are routinely employed in making environmental resource management decisions. The model supporting these decisions must be scientifically defensible and decision-makers must be informed of the degree of uncertainty in the model predictions. This has prompted some state agencies to develop standards for groundwater modeling. This guide provides a consistent framework within which to develop, apply, and document a groundwater flow model.

This guide presents steps ideally followed whenever a groundwater flow model is applied. The groundwater flow model will be based upon a mathematical model that may use numerical, analytical, or any other appropriate technique. This guide should be used by practicing groundwater modellers and by those wishing to provide consistency in modeling efforts performed under their direction.

There are limitations to the application of this guide. For example, development of an equivalent porous media model in karst terrain may not be valid if significant groundwater flow takes place in fractures and solution channels. In this case, the modeller could follow all steps in this guide and not end up with a defensible model.

This guide covers the application and subsequent documentation of a groundwater flow model to a particular site or problem. In this context, “groundwater flow model” refers to the application of a mathematical model to the solution of a site-specific groundwater flow problem.

ASTM E1689 - 95(2014), Standard Guide for Developing Conceptual Site Models for Contaminated Sites

Summary:

The information gained through the site investigation is used to characterize the physical, biological, and chemical systems existing at a site. The processes that determine contaminant releases, contaminant migration, and environmental receptor exposure to contaminants are described and integrated in a conceptual site model.

This guide is intended to assist in the development of conceptual site models to be used for the following: (1) integration of technical information from various sources, (2) support the selection of sample locations for establishing background concentrations of substances, (3) identify data needs and guide data collection activities, and (4) evaluate the risk to human health and the environment posed by a contaminated site. This guide generally describes the major components of conceptual site models, provides an outline for developing models, and presents an example of the parts of a model. This guide does not provide a detailed description of a site-specific conceptual site model because conditions at contaminated sites can vary greatly from one site to another.

ASTM D6025 - 96(2008), Standard Guide for Developing and Evaluating Groundwater Modeling Codes

Summary:

Groundwater modeling has become an important methodology in support of the planning and decision-making processes involved in groundwater management. Groundwater models provide an analytical framework for obtaining an understanding of the mechanisms and controls of groundwater systems and the processes that influence their quality, especially those caused by human intervention in such systems. Increasingly, models are an integral part of water resources assessment, protection, and restoration studies and provide essential and cost-effective support for planning and screening of alternative policies, regulations, and engineering designs affecting groundwater. It is therefore important that before groundwater modeling codes are used as planning and decision-making tools, their credentials are established and their suitability determined through systematic evaluation of their correctness, performance characteristics, and applicability. This becomes even more important because of the increasing complexity of the hydrologic systems for which new modeling codes are being developed.

Quality assurance in groundwater modeling provides the mechanisms and framework to ensure that the analytic tools used in preparing decisions are based on the best available techniques and methods. A well-executed quality assurance program in groundwater modeling provides the information necessary to evaluate the reliability of the performed analysis and the level to which the resulting advice may be incorporated in decision-making regarding the management of groundwater resources.

This guide is intended to encourage consistency and completeness in the development and evaluation of existing and new groundwater modeling codes by describing appropriate code development and quality assurance procedures and techniques.

This guide covers a systematic approach to the development, testing, evaluation, and documentation of groundwater modeling codes. The procedures presented constitute the quality assurance framework for a groundwater modeling code. They include code review, testing, and evaluation using quantitative and qualitative measures. This guide applies to both the initial development and the subsequent maintenance and updating of groundwater modeling codes.

ASTM D6170 - 97(2010), Standard Guide for Selecting a Groundwater Modeling Code

Summary:

Many different groundwater modeling codes are available, each with their own capabilities, operational characteristics and limitations. Furthermore, each groundwater project has its own requirements with respect to modeling. Therefore, it is important that the most appropriate code is selected for a particular project. This is even more important for projects that require extensive modeling, or where costly decisions are based, in part, on the outcome of modeling-based analysis.

Systematic and comprehensive description of project requirements and code features provides the necessary basis for efficient selection of a groundwater modeling code. This standard guide is intended to encourage comprehensive and consistent description of code capabilities and code requirements in the code selection process, as well as thorough documentation of the code selection process.

This guide covers a systematic approach to the determination of the requirements for and the selection of computer codes used in a groundwater modeling project. Due to the complex nature of fluid flow and biotic and chemical transport in the subsurface, many different groundwater modeling codes exist, each having specific capabilities and limitations. Furthermore, a wide variety of situations may be encountered in projects where groundwater models are used. Determining the most appropriate code for a particular application requires a thorough analysis of the problem at hand and the required and available resources, as well as detailed description of the functionality of candidate codes.

ASTM D5610 - 94(2014), Standard Guide for Defining Initial Conditions in Groundwater Flow Modeling

Summary:

Accurate definition of initial hydrologic conditions is an essential part of conceptualizing and modeling transient groundwater flow, because results of a simulation may be heavily dependent upon the initial conditions.

This guide covers techniques and procedures used in defining initial conditions for modeling saturated groundwater flow. The specification of initial conditions is an essential part of conceptualizing and modeling groundwater systems.

This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.

ASTM D5609 - 94(2016), Standard Guide for Defining Boundary Conditions in Groundwater Flow Modeling

Summary:

Accurate definition of boundary conditions is an essential part of conceptualizing and modeling groundwater flow systems. This guide describes the properties of the most common boundary conditions encountered in groundwater systems and discusses major aspects of their definition and application in groundwater models. It also discusses the significance and specification of boundary conditions for some field situations and some common errors in specifying boundary conditions in groundwater models.

This guide covers the specification of appropriate boundary conditions that are an essential part of conceptualizing and modeling groundwater systems. This guide describes techniques that can be used in defining boundary conditions and their appropriate application for modeling saturated groundwater flow model simulations. This guide is one of a series of standards on groundwater flow model applications. Defining boundary conditions is a step in the design and construction of a model that is treated generally in Guide D5447.

ASTM D5611 - 94(2016), Standard Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application

Summary:

After a model has been calibrated and used to draw conclusions about a physical hydrogeologic system (for example, estimating the capture zone of a proposed extraction well), a sensitivity analysis can be performed to identify which model inputs have the most impact on the degree of calibration and on the conclusions of the modeling analysis.

This guide covers techniques that should be used to conduct a sensitivity analysis for a groundwater flow model. The sensitivity analysis results in quantitative relationships between model results and the input hydraulic properties or boundary conditions of the aquifers.

After a groundwater flow model has been calibrated, a sensitivity analysis may be performed. Examination of the sensitivity of calibration residuals and model conclusions to model inputs is a method for assessing the adequacy of the model with respect to its intended function.

ASTM D5490 - 93(2014)e1, Standard Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information

Summary:

During the process of calibration of a groundwater flow model, each simulation is compared to site-specific information to ascertain the success of previous calibration efforts and to identify potentially beneficial directions for further calibration efforts. Procedures described herein provide guidance for making comparisons between groundwater flow model simulations and measured field data.

This guide covers techniques that should be used to compare the results of groundwater flow model simulations to measured field data as a part of the process of calibrating a groundwater model. This comparison produces quantitative and qualitative measures of the degree of correspondence between the simulation and site-specific information related to the physical hydrogeologic system.

ASTM D5718 - 13, Standard Guide for Documenting a Groundwater Flow Model Application

Summary:

Groundwater flow models are tools frequently applied for the analysis of hydrogeologic systems. Due to the significance of many decisions based upon modeling results, quality assurance measures need to be applied to model applications. Complete model documentation is a mechanism to ensure the quality of the effort. Several federal and state agencies have developed policies regarding model documentation. This guide provides consistency amongst current policies, and should be used as a framework for model documentation.

This guide covers suggested components to be included in documenting and archival of numerical groundwater flow model applications. Model documentation includes a written and graphical presentation of model assumptions and objectives, the conceptual model, code description, model construction, model calibration, predictive simulations, and conclusions. Model archival refers to a file or set of files (in both written and digital format) that contains logs of significant model simulations (that is, calibration, sensitivity and prediction simulations), supplemental calculations, model documentation, a copy of the model source code(s) or executable file(s) used, or both, and input and output data sets for significant model simulations.

Although the ASTM documents are relatively complete in covering all aspects of groundwater modelling, practitioners have found that the standards are sometimes out of date and at a level below that of current practice achieved by leading government agencies (e.g., United States Geological Survey) and specialist consultants. Therefore, the following reference list provides other materials that can be helpful guides for groundwater modelling.

Groundwater modelling textbooks

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

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Wels, C., D. Mackie, and J. Scibek, 2012: Guidelines for Groundwater Modelling to Assess Impacts of Proposed Natural Resource Development Activities; prepared by Robertson GeoConsultants Inc. and SRK Consulting for the British Columbia Ministry of the Environment, Water Protection & Sustainability Branch.

Groundwater monographs on groundwater modelling

Franke, O.L., T.E. Reilly, and G.D. Bennett, 1987: Definition of boundary and initial conditions in the analysis of saturated ground-water flow systems – an introduction; United States Geological Survey, Techniques of Water-Resources Investigations, Book 3, Chapter B5.

Hill, M.C., 1998: Methods and guidelines for effective model calibration; with application to UCODE, a computer code for universal inverse modeling, and MODFLOWP, a computer code for inverse modeling with MODFLOW; United States Geological Survey, Water-Resources Investigations Report 98-4005.

Reilly, T.E., 2001: System and boundary conceptualization in ground-water flow simulation; United States Geological Survey, Techniques of Water-Resources Investigations, Book 3, Chapter B8.

Reilly, T.E. and A.W. Harbaugh, 2004: Guidelines for evaluating ground-water flow models; United States Geological Survey, Scientific Investigations Report 2004-5038.

Reilly, T.E., O.L. Franke, and G.D. Bennett, 1987: The principle of superposition and its application in ground-water hydraulics; United States Geological Survey, Techniques of Water-Resources Investigations, Book 3, Chapter B6.

Other groundwater references

Hill, M.C., H. Middlemis, P. Hulme, E. Poeter, J. Riegger, S.P. Neuman, H. Williams, and M. Anderson, 2004: Brief overview of selected groundwater modelling guidelines; *in* Proceedings of Finite-Element Models, MODFLOW, and More Conference, K. Kovar, Z. Hrkal, and J. Bruthans (eds.), Karlovy Vary, Czech Republic, p.105–120.

Schween, R.E. and S.P. Larson, 1986: Groundwater modeling: capabilities and limitations, use and abuse; Chapter 22 *in* the Proceedings of the Thirty-Second Annual Institute, Rocky Mountain Mineral Law Institute, Times Mirror Books.

van der Heijde, P.K.M., 1986: Quality assurance in computer simulations of groundwater contamination; Environmental Software, v.2, no.1, p.19–25.

Willing, P., 2007: A Nontechnical Guide to Groundwater Modeling; Natural Resources Defense Council, New York, New York.

1.2 Guidelines on Good Modelling Practices for Hydrological Modelling

Guidelines on good modelling practices are aimed at ensuring model results that are “accurate, practical and reproducible” (State of Arizona, 2007b, p.102). Such guidelines are not aimed at the organizational process of managing modelling processes or maintaining the knowledge about models over time, but they provide a technical framework for the selection of input data, calibration, model uncertainty assessment, evaluation, documentation, and communication of results. Two key points provided in a guideline relate to i) reproducibility of results, and ii) practicality. The State of Arizona (2007b, p.102), for example, defines reproducibility as “a measure of the degree of interpretation required to implement a guideline. Reproducibility is generally achieved through clear and concise procedures”. In the guideline, practicality takes into account the following considerations:

- anticipated user,
- current technology being applied,
- availability of data,
- ability to simulate a range of hydrologic conditions,
- consequences of error, and
- desired output.

A number of guidelines on good modelling practices were reviewed and are presented under the following subsections: general hydrology, rainfall-runoff modelling, flood forecasting and watershed modelling, water quality modelling, urban water cycle systems, and groundwater–surface water interactions.

1.2.1 General Hydrology

Refsgaard, J.C. and H.J. Henriksen, 2004: Modelling guidelines—terminology and guiding principles; Advances in Water Resources, v.27, no.1, p.71–82.

Abstract:

Some scientists argue, with reference to Popper’s scientific philosophical school, that models cannot be verified or validated. Other scientists and many practitioners nevertheless use these terms, but with very different meanings. As a result of an increasing number of examples of model malpractice and mistrust in the credibility of models, several modelling guidelines have been enhanced in recent years with the broad aim of improving the quality of modelling studies. This gap between these views and the lack of consensus in the scientific community coupled with the strongly perceived need for commonly agreed upon modelling guidelines is constraining the optimal use and benefits of models. This paper proposes a framework for quality assurance guidelines, including a consistent terminology and a foundation for a methodology that bridges the gap between scientific philosophy and pragmatic modelling. A distinction is made between the conceptual model, the model code and the site-specific model. A conceptual model is subject to confirmation or falsification, in a similar fashion to scientific theories. A model code may be verified within given ranges of applicability and ranges of accuracy, but it can never be universally verified. Similarly, a model may be validated, but only with reference to site-specific applications and to pre-specified performance (accuracy) criteria. Thus, a model’s validity will always be limited in terms of space, time, boundary conditions and types of application. This implies a continuous interaction between manager and modeller in order to establish suitable accuracy criteria and predictions associated with uncertainty analysis.

Moriasi, D.N., J.G. Arnold, M.W. Van Liew, R.L. Bingner, R.D. Harmel, and T.L. Veith, 2007: Model evaluation guidelines for systematic quantification of accuracy in watershed simulations; Transactions of the ASABE, v.50, no.3, p.885–900.

Abstract:

Watershed models are powerful tools for simulating the effect of watershed processes and management on soil and water resources. However, no comprehensive guidance is available to facilitate model evaluation in terms of the accuracy of simulated data compared to measured flow and constituent values. Thus, the objectives of this research were to: (1) determine recommended model evaluation techniques (statistical and graphical), (2) review reported ranges of values and corresponding performance ratings for the recommended statistics, and (3) establish guidelines for model evaluation based on the review results and project-specific considerations; all of these objectives focus on simulation of streamflow and transport of sediment and nutrients. These objectives were achieved with a thorough review of relevant literature on model application and recommended model evaluation methods. Based on this analysis, we recommend that three quantitative statistics, Nash-Sutcliffe efficiency (NSE), percent bias (PBIAS), and ratio of the root mean square error to the standard deviation of measured data (RSR), in addition to the graphical techniques, be used in model evaluation. The following model evaluation performance ratings were established for each recommended statistic. In general, model simulation can be judged as satisfactory if NSE >0.50 and RSR <0.70, and if PBIAS + 25% for streamflow, PBIAS + 55% for sediment, and PBIAS + 70% for N and P. For PBIAS, constituent-specific performance ratings were determined based on uncertainty of measured data. Additional considerations related to model evaluation guidelines are also discussed. These considerations include: single-event simulation, quality and quantity of measured data, model calibration procedure, evaluation time step, and project scope and magnitude. A case study illustrating the application of the model evaluation guidelines is also provided.

Beven, K., 2006: A manifesto for the equifinality thesis; Journal of Hydrology, v.320, no.1, p.18–36.

Abstract:

This essay discusses some of the issues involved in the identification and predictions from hydrological models given calibration data. The reasons for the incompleteness of traditional calibration methods are discussed. An argument is made that the potential for multiple acceptable models as being reflective of hydrological and other environmental systems (i.e. the equifinality thesis) should be given more serious consideration than hitherto. It proposes some techniques for an extended GLUE methodology to make it more rigorous and outlines some of the research issues that still need to be resolved.

Beven, K. and P. Young, 2013: A guide to good practice in modeling semantics for authors and referees; Water Resources Research, v.49, no.8, p.5092–5098.

Abstract:

This opinion piece makes some suggestions regarding modeling semantics that can be used by authors and referees. Descriptions of model structures, different forms of simulation and prediction, different sources of uncertainty in modeling practice, the language of model validation, and the concepts of predictability and fitness-for-purpose are discussed. While not expecting universal agreement on these suggestions, given the loose usage of words in the literature, it is hoped that the discussion of the issues involved will at least give pause for thought and encourage good practice in model development and applications.

Black, D., P. Wallbrink, P. Jordan, D. Waters, C. Carroll, and J. Blackmore, 2011: Guidelines for Water Management Modelling: Towards Best-Practice Model Application; eWater Cooperative Research Centre, Bruce, Australia.

Summary:

The eWater CRC has prepared these generic best practice modelling guidelines that aim to provide for an integrated approach that enables interactions and feedbacks between all domains relevant to water management (e.g. hydrological, ecological, engineering, social, economic and environmental) to be considered.

Procedures are intended to be sufficiently flexible to accommodate variations in the meaning of the term "Best Practice Modelling" and to also allow for continuous improvement as the state of knowledge and technology in the modelling field develops and improves.

Harmel, R.D., P.K. Smith, K.W. Migliaccio, I. Chaubey, K.R. Douglas-Mankin, B. Benham, S. Shukla, R. Muñoz-Carpena, and B.J. Robson, 2014: Evaluating, interpreting, and communicating performance of hydrologic/water quality models considering intended use: a review and recommendations; Environmental Modelling & Software, v.57, p.40–51.

Summary:

This position paper provides an overview on the evaluation, interpretation, and communication of model performance for different governance purposes. Based on combinations of three dimensions of uncertainty i) error in model prediction ("model accuracy"); ii) the availability and quality of data ("data uncertainty"); and iii) structural model uncertainty ("model uncertainty"), the authors give recommendations for model interpretation and refinement for Exploratory, Planning, and Regulatory/Legal phases of modelling studies.

Abstract:

Previous publications have outlined recommended practices for hydrologic and water quality (H/WQ) modeling, but limited guidance has been published on how to consider the project's purpose or model's intended use, especially for the final stage of modeling applications – namely evaluation, interpretation, and communication of model results. Such guidance is needed to more effectively evaluate and interpret model performance and more accurately communicate that performance to decision-makers and other modeling stakeholders. Thus, we formulated a methodology for evaluation, interpretation, and communication of H/WQ model results. The recommended methodology focuses on interpretation and communication of results, not on model development or initial calibration and validation, and as such it applies to the modeling process following initial calibration. The methodology recommends the following steps: 1) evaluate initial model performance; 2) evaluate outliers and extremes in observed values and bias in predicted values; 3) estimate uncertainty in observed data and predicted values; 4) re-evaluate model performance considering accuracy, precision, and hypothesis testing; 5) interpret model results considering intended use; and 6) communicate model performance. A flowchart and tables were developed to guide model interpretation, refinement, and proper application considering intended model uses (i.e., *Exploratory*, *Planning*, and *Regulatory*/*Legal*). The methodology was designed to enhance application of H/WQ models through conscientious evaluation, interpretation, and communication of model performance to decision-makers and other stakeholders; it is not meant to be a definitive standard or a required protocol, but together with recent recommendations and published best practices serve as guidelines for enhanced model application emphasizing the importance of the model's intended use.

Rassam, D., I. Jolly, and T. Pickett, 2011: Guidelines for Modelling Groundwater-Surface Water Interactions in eWater Source: Towards Best Practice Model Application; eWater Cooperative Research Centre, Bruce, Australia, Interim version 1.0.

Summary:

These high level guidelines provide a generic procedure for delivering high quality modelling outcomes. The document is not meant to be prescriptive, nor to re-invent material and concepts that are available elsewhere and therefore draws on material available from the international literature and on the internet. A generic modelling procedure, comprised of four steps i) project management; ii) problem definition; iii) option modelling; and iv) option comparison, is put forward to support best modelling practices.

1.2.2 Rainfall-Runoff Modelling

Vaze, J., P. Jordan, R. Beecham, A. Frost, and G. Summerell, 2011: Guidelines for Rainfall-Runoff Modelling: Towards Best Practice Model Application; eWater Cooperative Research Centre, Bruce, Australia, Interim version 1.0.

Summary:

The eWater CRC will also provide guidance to support the BPM guidelines in specific areas of hydrological modelling that relate to the products that they are developing. This guideline is intended to address rainfall-runoff model applications with the objectives being to provide water managers, consultants and research scientists with information on rainfall-runoff models and how to choose one that is fit for purpose, the data available to develop them, and the calibration and validation methodologies.

Barma, D. and I. Varley, 2012: Hydrological Modelling Practices for Estimating Low Flows–Guidelines; Australian Government, National Water Commission.

Summary:

These guidelines promote best practice in estimating low flows, including cease-to-flow, in rainfall-runoff and river system models. The document provides advice pertaining to data considerations, model selection, model configuration and model calibration strategies. A key contribution is the discussion on approaches to estimating flows in ungauged catchments. The document draws on existing modelling practices in Australia and highlights specific case studies to test a number of the recommended methodologies. The guideline complements the more extensive suite of eWater modelling guideline documents.

1.2.3 Flood Forecasting and Watershed Modelling

Marsh, N., F. Sheldon, P. Wettin, C. Taylor, and D. Barma, 2012: Guidance on ecological responses and hydrological modelling for low-flow water planning; Australian Government, National Water Commission.

Summary:

This report assists with ecological response and hydrological modelling considerations in low-flow water planning by summarising the outcomes of six key reports generated by two "low flows" projects commissioned by the National Water Commission. To make the information in the reports more accessible to water planners and managers, it is organised around the seven typical steps in a water planning process as identified in the draft *NWI Policy Guidelines for Water Planning and Management*.

Moore, R.J., V.A. Bell, S.J. Cole, and D.A. Jones, 2007*:* Rainfall-runoff and other modelling for ungauged/low-benefit locations: operational guidelines; Environment Agency, Bristol, United Kingdom, Science Report – SC030227/SR2.

Summary:

Across England and Wales, the Environment Agency provides only a general "Flood Watch" (as opposed to a higher level "Flood Warning") service at ungauged locations where benefit of a higher level service would be marginal. To provide an improved, more targeted "Flood Warning" service in these locations, this document discusses current best practices and identifies future research opportunities.

Against this background, this report provides an overview of approaches for modelling at ungauged locations to guide operational practice both now and in the future. It also serves as a "roadmap" to an accompanying Science Report where more detail can be found. The emphasis is on the types of modelling problems commonly encountered and the general approaches that can be considered when addressing them. Whilst rainfall-runoff models are the main focus of attention, broader discussion encompasses hydrological channel flow routing models and hydrodynamic river models; simpler empirical models including level-to-level correlation methods are also considered.

State of Arizona, 2007a: State Standard for Hydrologic Modeling Guidelines; Arizona Department of Water Resources - Flood Mitigation Section, SS10-07.

Summary:

State Standard for Hydrological Modeling has been developed to address hydrologic conditions for a variety of Arizona watersheds. Included are problems and situations identified by the State Standard Work Group (SSWG) and floodplain managers. The intended audience includes Arizona's engineers, associated professionals and Floodplain Administrators. Case studies that address the following topics are included:

- Hydrologic Model comparison and recommendation
- Guidelines and parameters
- Model application for specific situations, and associated hydrologic parameters
- Precipitation values (NOAA 14)
- Storm duration
- Unique conditions, such as wildfire burn, overgrazing, logging, drought, rapid snowmelt, urbanization.

State of Arizona, 2007b: State Standard for Hydrologic Modeling Guidelines - Technical Supplement*; Arizona Department of Water Resources - Flood Mitigation Section, Appendix 1, SS10-07 Supplement.*

Summary:

This technical supplement contains Introduction and Purpose, Literature Search & Data Collection, Agency Contacts, Floodplain Management Survey, and a list of Hydrologic Models that meet the requirements of the National Flood Insurance Program (NFIP). A summary of hydrological modelling guidelines is included. The document is very technical in nature.

1.2.4 Water Quality Modelling

Moriasi, D.N., B.N. Wilson, K.R. Douglas-Mankin, J.G. Arnold, and P.H. Gowda, 2012: Hydrologic and water quality models: use, calibration, and validation; Transactions of the ASABE, v.55, no.4, p.1241–1247.

Summary:

To provide a common background and platform for consensual development of calibration and validation guidelines, model developers and/or expert users of commonly used hydrologic and water quality models were invited to write technical articles recommending model specific calibration and validation procedures. This article introduces a collection of 22 research articles that present and discuss calibration and validation concepts in detail for 25 hydrologic and water quality models. The main objective of this article is to introduce and summarize key aspects of the hydrologic and water quality models presented in this collection. The models range in scale from field to watershed and simulate various processes including hydrology, sediment, nutrients, bacteria, and pesticides at temporal scales varying from hourly to annually. The articles provide model practitioners with detailed, model-specific guidance on model calibration, validation, and use. Collectively, the articles in this collection present a consistent framework of information that will facilitate development of a proposed set of ASABE model calibration and validation guidelines.

Wang, Q., S. Li, P. Jia, C. Qi, and F. Ding, 2013: A review of surface water quality models; The Scientific World Journal, v.2013, Article ID 231768.

Abstract:

Surface water quality models can be useful tools to simulate and predict the levels, distributions, and risks of chemical pollutants in a given water body. Model results, under varying pollution scenarios, provide important inputs to environmental impact assessment studies and can provide baseline technical support for environmental management agency decisions. The reliance on model results can significantly impact the defensibility of authorized construction projects and the possible implementation of pollution control measures. The development of surface water quality models at three stages was reviewed and the authors analyzed the suitability, precision, and methods of different models. Standardization of water quality models can help environmental management agencies guarantee consistency in model application for regulatory purposes. The standardization of surface water quality models is recommended and standardization measures, particularly within developing countries, are put forward.

1.2.5 Urban Water Cycle Systems

Monteiro, A.J., A. Fonseca Galvão, J. Martins Pisoeiro, and P. Ribeiro, 2015: Guidelines for Assessment of Urban Water Cycle Systems Current Situation and Future Scenarios; Transitions to Urban Water Services for Tomorrow (TRUST), D51.2.

Abstract:

To establish a management strategy for transitioning to a more sustainable Urban Water Cycle Systems (UWCS), water utilities need to identify: i) the current state of the UWCS they manage; ii) possible future scenarios; and iii) a preliminary portfolio of possible transition pathways. These guidelines are a useful tool developed with the purpose of logically assisting urban water utilities in characterizing and evaluating the current status and in defining possible scenarios and tracks that can be taken by utilities to transition to more sustainable urban water management systems. The guidelines were designed to introduce and drive practitioners (water professionals, decision makers, stakeholders) to the use of "TRUST" deliverables, or to use other identified best approaches. The guidelines consist of a portfolio of "Situation Analysis Factsheets (SAF)" developed for each "TRUST" deliverable. Each SAF synthesizes the following information into no more than two pages: i) framework scheme of the tool; ii) purpose and output; iii) objectives and main output; iv) inputs and resources; v) data, human resources and time needed; vi) methodology; vii) approach; viii) disadvantages/limitations; and ix) links to additional information. Finally, a matrix identifying sustainability dimensions; the capability for analyzing current and/or future situations; the relation with the TRUST criteria; and objectives for each tool/approach is provided in the Situation Analysis Factsheet.

1.2.6 Groundwater–Surface Water Interactions

Refsgaard, J.C., A.L. Højberg, I. Møller, M. Hansen, and V. Søndergaard, 2010: Groundwater modeling in integrated water resources management—visions for 2020; Ground Water, v.48, no.5, p.633-648.

Abstract:

Groundwater modeling is undergoing a change from traditional stand-alone studies, towards studies where groundwater modelling is one integrated component of a more holistic water resource management approach. This is illustrated by developments in Denmark, where comprehensive national databases for geologic borehole data, groundwater-related geophysical data, geologic models, as well as national groundwater-surface water models have been established and integrated to support water management. This has enhanced the benefits of

using groundwater models. Based on insight gained from this Danish experience, a scientifically realistic scenario for the use of groundwater modeling in 2020 has been developed, in which groundwater models will be a part of sophisticated databases and modeling systems. The databases and numerical models will be seamlessly integrated, and the tasks of monitoring and modeling will be merged. Numerical models for atmospheric, surface water, and groundwater processes will be coupled in one integrated modeling system that can operate at a wide range of spatial scales. Furthermore, the management systems will be constructed with a focus on building credibility of model and data use among all stakeholders and on facilitating a learning process whereby data and models, as well as stakeholders' understanding of the system, are updated with currently available information. The key scientific challenges for achieving this 2020 vision are: (1) developing new methodologies for integration of statistical and qualitative uncertainty; (2) mapping geological heterogeneity and developing scaling methodologies; (3) developing coupled model codes; and (4) developing integrated information systems, including quality assurance and uncertainty information that facilitates active stakeholder involvement and learning.

Rassam, D., I. Jolly, and T. Pickett, 2011: Guidelines for Modelling Groundwater-Surface Water Interactions in eWater Source: Towards Best Practice Model Application; eWater Cooperative Research Centre, Bruce, Australia, Interim version 1.0.

Summary:

This document provides initial guidance on applying GW-SW [groundwater-surface water] interactions in existing river and groundwater models, with specific applicability to the “Source” Integrated Modelling System which incorporates GW-SW functionality. It is based on a combination of a literature review, as well as lessons learned from work undertaken in the Murray-Darling and Namoi River Basins.

The target audience for this document is practising river system and catchment modellers who are interested in incorporating GW-SW interactions in their river planning models, i.e. it is not a text book. The document is one of a series of Best Practice Modelling documents prepared by eWater.

1.3 Guidelines for Integrated Environmental Modelling

Beck, M.B., 2009: Grand challenges of the future for environmental modeling; National Science Foundation, Arlington, Virginia, White Paper.

Abstract:

This White Paper sets out thirteen Grand Challenges of the future for environmental modeling in response to that question. The same grand challenges are also set out in the Synopsis of this Paper, which is available as a separate document and which can be read as an extended Executive Summary of the present document. Both the Synopsis and this White Paper introduce and discuss each challenge in the same format: of the context and foundations of — hence, the justification of — why each should have been identified as a challenge in the contemporary research scene; followed by expression of the challenge itself; with then a discussion of some indicative lines of possible responses to the challenge. While composition of this White Paper has been prompted by the EO initiatives, our grand challenges have been evolving over the years, and will endure into the future, irrespective of the substantial current commitments to plans for realizing the ambitions of the Observatories. They therefore merit significant consideration as matters for further research in their own right.

Jakeman, A.J., R.A. Letcher, and J.P. Norton, 2006: Ten iterative steps in development and evaluation of environmental models; Environmental Modelling & Software, v.21, no.5, p.602–614.

Summary:

With over 550 citations, this position paper has remained one of the most downloaded papers and is still considered a standard paper on the process of performing environmental modelling studies. The ten steps presented here should be executed in consort with end-users, with every stage open to critical review and revision. The authors have observed that too often, it is common practice to apply predetermined concepts to model a given situation. By highly constricting the modelling of a problem to strong assumptions of the modeller, predicted outcomes and policy recommendations simply reproduce the dominant opinion. The proposed 10 steps are meant to ensure that a model accurately takes into consideration all potential cause-effect mechanisms of a problem, requiring multiple disciplines at the table.

Abstract:

Models are increasingly being relied upon to inform and support natural resource management. They are incorporating an ever broader range of disciplines and now often confront people without strong quantitative or model-building backgrounds. These trends imply a need for wider awareness of what constitutes good model-development practice, including reporting of models to users and sceptical review of models by users. To this end the paper outlines ten basic steps of good, disciplined model practice. The aim is to develop purposeful, credible models from data and prior knowledge, in consort with end-users, with every stage open to critical review and revision. Best practice entails identifying clearly the clients and objectives of the modelling exercise; documenting the nature (quantity, quality, limitations) of the data used to construct and test the model; providing a strong rationale for the choice of model family and features (encompassing review of alternative approaches); justifying the techniques used to calibrate the model; serious analysis, testing and discussion of model performance; and making a resultant statement of model assumptions, utility, accuracy, limitations, and scope for improvement. In natural resource management applications, these steps will be a learning process, even a partnership, between model developers, clients and other interested parties.

Crout, N., T. Kokkonen, A.J. Jakeman, J.P. Norton, L.T.H. Newham, R. Anderson, H. Assaf, B.F.W. Croke, N. Gaber, J. Gibbons, D. Holzworth, J. Mysiak, J. Reichl, R. Seppelt, T. Wagener, and P. Whitfield, 2008: Chapter two, good modelling practice; *in* Environmental Modelling, Software and Decision Support: State of the Art and New Perspectives, A.J. Jakeman, A.A. Voinov, A.E. Rizzoli, and S.H. Chen (eds.), Developments in Integrated Environmental Assessment, v.3, p.15–31.

Abstract:

Models have become indispensable in environmental assessment, planning and management. However as models have increasingly been developed and disseminated, the risk of their misuse or misunderstanding of their capabilities has increased. Whether a model is used for simulation, prediction, decision making or communication of scientific analyses, it is important that its

development and application conform to protocols or standards that help to maximise the scientific soundness, utility and defensibility of models and their outputs. The complexity and uncertainty inherent in environmental assessment make the pursuit of good modelling practice especially important, in spite of limited time and resources. This paper is an attempt to identify the key components of best modelling practice and our collective progress in its achievement, taking into account previous relevant reviews undertaken by several authors and agencies. The details are always likely to be the subject of lively debate, but the general components of 'good modelling practice' are probably not controversial. They are clear purpose, adequate reporting, and serious evaluation. Although these are common strands in the various definitions of good modelling practice the emphasis varies between different types of model application. For this reason it is important that good practice should not become overly prescriptive.

We report a preliminary analysis which suggests that progress towards improving modelling practice is slow. This is despite very widespread agreement on what constitutes good practice. Why is this so? In the research community at least, the drivers for model development and evaluation are funding and publication. If modelling practice needs to be improved, and we think it does, sponsors and journals need to take a lead in creating an environment where developing a model requires that the work be undertaken under some system of good modelling practice. The suggestion has been made of a 'good practice check list' in the journal, Environmental Modelling and Software. While such a system would need to be flexibly applied, the principle is sound, and such steps should move us forward.

Scholten, H., A. Kassahun, J.C. Refsgaard, T. Kargas, C. Gavardinas, and A.J. Beulens, 2007: A methodology to support multidisciplinary model-based water management; Environmental Modelling & Software v.22, no.5, p.743–759.

Abstract:

Quality assurance in model based water management is needed because of some frequently perceived shortcomings, e.g. a lack of mutual understanding between modelling team members, malpractice and a tendency of modellers to oversell model capabilities. Initiatives to support quality assurance focus on single domains and often follow a textbook approach with guidelines and checklists. A modelling process involves a complex set of activities executed by a team. To manage this complex, usually multidisciplinary process, to guide users through it and enhance the reproducibility of modelling work a software product has been developed, aiming at supporting the full modelling process by offering an ontological knowledge base (KB) and a Modelling Support Tool (MoST). The KB consists of a generic part for modelling, but also parts specific for various water management domains, for different types of users and for different levels of modelling complexity. MoST's guiding component filters relevant knowledge from the KB depending on the user profile and needs. Furthermore, MoST supports different types of users by monitoring what they actually do and by producing customized reports for diverse audiences. In this way MoST facilitates co-operation in teams, modelling project audits and re-use of experiences of previous modelling projects.

Bennett, N.D., B. Croke, G. Guariso, J. Guillaume, S. Hamilton, A. Jakeman, and S. Marsili-Libelli, 2013: Characterising performance of environmental models; Environmental Modelling & Software, v.40, p.1–20.

Abstract:

In order to use environmental models effectively for management and decision-making, it is vital to establish an appropriate level of confidence in their performance. This paper reviews techniques available across various fields for characterising the performance of environmental models with focus on numerical, graphical and qualitative methods on parameter values and data transformations:

- direct value comparison (e.g. mean, median, variance, skew, curtosis, histogram, frequency distribution plot),
- comparing real and modelled values (e.g. scatter plots, regression analysis, bias score, probability of detection, other statistics),
- residual methods with and without data transformations (e.g. residual plot, (root) mean square error, relative bias, log transformed root mean, heteroscedastic maximum likelihood estimator),
- data pattern preservation and model efficiency performance measures (e.g. correlations, cross-correlations, Nash-Sutcliffe Model Efficiency, Index of Agreement, Relative Absolute Error),
- indirect metrics (e.g. average relative parameter error, Akaike Information Criterion), and
- data transformation methods (e.g. Fourier transform and power spectral density, Wavelet transformation, Empirical orthogonal functions).

In practice environmental modelling requires the use and implementation of workflows that combine several methods, tailored to the model purpose and dependent upon the data and information available. A five-step procedure for performance evaluation of models is suggested, with the key elements including: (i) (re)assessment of the model's aim, scale and scope; (ii) characterisation of the data for calibration and testing; (iii) visual and other analysis to detect under- or non-modelled behaviour and to gain an overview of overall performance; (iv) selection of basic performance criteria; and (v) consideration of more advanced methods to handle problems such as systematic divergence between modelled and observed values.

McIntosh, B.S., J.C. Ascough, M. Twery, J. Chew, A. Elmahdi, D. Haase, and J.J. Harou, 2011: Environmental decision support systems (EDSS) development–challenges and best practices; Environmental Modelling & Software, v.26, no.12, p.1389–1402.

Abstract:

Despite the perceived value of DSS in informing environmental and natural resource management, DSS tools often fail to be adopted by intended end users. By drawing together the experience of a global group of EDSS developers, we have identified and assessed key challenges in EDSS development and offer recommendations to resolve them. Challenges related to engaging end users in EDSS development emphasise the need for a participatory process that embraces end users and stakeholders throughout the design and development process. Adoption challenges concerned with individual and organisational capacities to use EDSS and the match between EDSS and organisational goals can be overcome through the use of an internal champion to promote the EDSS at different levels of a target organisation; co-ordinate and build capacity within the organisation, and ensure that developers maintain focus on developing EDSS which are relatively easy and inexpensive to use and update (and which are perceived as such by the target users). Significant challenges exist in relation to ensuring EDSS longevity and financial sustainability. Such business challenges may be met through planning and design that considers the long-term costs of training, support, and maintenance; revenue generation and licensing by instituting processes which support communication and interactions; and by employing software technology which enables easy model expansion and re use to gain an economy of scale and reduce development costs. A final group of perhaps more problematic challenges relate to how the success of EDSS ought to be evaluated. Whilst success can be framed relatively easily in terms of interactions with end users, difficulties of definition and measurability emerge in relation to the extent to which EDSS achieve intended outcomes. To tackle the challenges described, the authors provide a set of best practice recommendations concerned with promoting design for ease of use, design for usefulness, establishing trust and credibility, promoting EDSS acceptance, and starting simple and small in functionality terms. Following these recommendations should enhance the achievement of successful EDSS adoption, but more importantly, help facilitate the achievement of desirable social and environmental outcomes.

Laniak, G.F., G. Olchin, J. Goodall, A. Voinov, M. Hill, P. Glynn, and G. Whelan, 2013: Integrated environmental modeling: a vision and roadmap for the future; Environmental Modelling & Software, v.39, p.3–23.

<u>*Abstract:*</u>

Integrated environmental modeling (IEM) is inspired by modern environmental problems, decisions, and policies and enabled by transdisciplinary science and computer capabilities that allow the environment to be considered in a holistic way. The problems are characterized by the extent of the environmental system involved, dynamic and interdependent nature of stressors and their impacts, diversity of stakeholders, and integration of social, economic, and environmental considerations. IEM provides a science-based structure to develop and organize relevant knowledge and information and apply it to explain, explore, and predict the behavior of environmental systems in response to human and natural sources of stress. During the past several years a number of workshops were held that brought IEM practitioners together to share experiences and discuss future needs and directions. In this paper we organize and present the results of these discussions. IEM is presented as a landscape containing four interdependent elements: applications, science, technology, and community. The elements are described from the perspective of their role in the landscape, current practices, and challenges that must be addressed. Workshop participants envision a global scale IEM community that leverages modern technologies to streamline the movement of science-based knowledge from its sources in research, through its organization into databases and models, to its integration and application for problem solving purposes. Achieving this vision will require that the global community of IEM stakeholders transcend social, and organizational boundaries and pursue greater levels of collaboration. Among the highest priorities for community action are the development of standards for publishing IEM data and models in forms suitable for automated discovery, access, and integration; education of the next generation of environmental stakeholders, with a focus on transdisciplinary research, development, and decision making; and providing a web-based platform for community interactions (e.g., continuous virtual workshops).

Hamilton, S.H., S. ElSawah, J. Guillaume, A. Jakeman, and S. Pierce, 2015: Integrated assessment and modelling: overview and synthesis of salient dimensions; Environmental Modelling & Software, v.64, p.215–229.

Abstract:

Integrated assessment and its inherent platform, integrated modelling, present an opportunity to synthesize diverse knowledge, data, methods and perspectives into an overarching framework to address complex environmental problems. However to be successful for assessment or decision making purposes, all salient dimensions of integrated modelling must be addressed with respect to its purpose and context. The key dimensions include: issues of concern; management options and governance arrangements; stakeholders; natural systems; human systems; spatial scales; temporal scales; disciplines; methods, models, tools and data; and sources and types of uncertainty. This paper aims to shed light on these ten dimensions, and how integration of the dimensions fits in the four main phases in the integrated assessment process: scoping, problem framing and formulation, assessing options, and communicating findings. We provide examples of participatory processes and modelling tools that can be used to achieve integration.

Voinov, A., N. Kolagani, M.K. McCall, P.D. Glynn, M.E. Kragt, F.O. Ostermann, S.A. Pierce, and P. Ramu, 2016: Modelling with stakeholders–next generation; Environmental Modelling & Software, v.77, p.196–220.

Abstract:

This paper updates and builds on 'Modelling with Stakeholders' Voinov and Bousquet, 2010 which demonstrated the importance of, and demand for, stakeholder participation in resource and environmental modelling. This position paper returns to the concepts of that publication and reviews the progress made since 2010. A new development is the wide introduction and acceptance of social media and web applications, which dramatically changes the context and scale of stakeholder interactions and participation. Technology advances make it easier to incorporate information in interactive formats via visualization and games to augment participatory experiences. Citizens as stakeholders are increasingly demanding to be engaged in planning decisions that affect them and their communities, at scales from local to global. How people interact with and access models and data is rapidly evolving. In turn, this requires changes in how models are built, packaged, and disseminated: citizens are less in awe of experts and external authorities, and they are increasingly aware of their own capabilities to provide inputs to planning processes, including models. The continued acceleration of environmental degradation and natural resource depletion accompanies these societal changes, even as there is a growing acceptance of the need to transition to alternative, possibly very different, life styles. Substantive transitions cannot occur without significant changes in human behaviour and perceptions. The important and diverse roles that models can play in guiding human behaviour, and in disseminating and increasing societal knowledge, are a feature of stakeholder processes today.

1.4 LESSONS FROM OTHER DISCIPLINES

In some related areas, first lessons already exist, for example, for workflow management in enterprises (Van der Aalst, 1998), environmental decision support software systems (McIntosh, 2011 – see above), or business process models in the corporate world (Koschmider and Reijers, 2015).

Hey, T., S. Tansley, and K.M. Tolle (eds.), 2009: The Fourth Paradigm: Data-Intensive Scientific Discovery; Microsoft Research, Redmond, Washington, URL <https://www.microsoft.com/en-us/research/publication/fourth-paradigm-data-intensive-scientific-discovery/>.

Abstract:

> Increasingly, scientific breakthroughs will be powered by advanced computing capabilities that help researchers manipulate and explore massive datasets.
>
> The speed at which any given scientific discipline advances will depend on how well its researchers collaborate with one another, and with technologists, in areas of eScience such as databases, workflow management, visualization, and cloud computing technologies.
>
> In *The Fourth Paradigm: Data-Intensive Scientific Discovery*, the collection of essays expands on the vision of pioneering computer scientist Jim Gray for a new, fourth paradigm of discovery based on data-intensive science and offers insights into how it can be fully realized.

Van der Aalst, W.M.P., 1998: The application of Petri nets to workflow management; Journal of Circuits, Systems and Computers, v.8, no.01, p.21–66, URL <http://www.worldscientific.com/doi/abs/10.1142/S0218126698000043>.

Abstract:

> Workflow management promises a new solution to an age-old problem: controlling, monitoring, optimizing and supporting business processes. What is new about workflow management is the explicit representation of the business process logic which allows for computerized support. This paper discusses the use of Petri nets in the context of workflow management. Petri nets are an established tool for modeling and analyzing processes. On the one hand, Petri nets can be used as a design language for the specification of complex workflows. On the other hand, Petri net theory provides for powerful analysis techniques which can be used to verify the correctness of workflow procedures. This paper introduces workflow management as an application domain for Petri nets, presents state-of-the-art results with respect to the verification of workflows, and highlights some Petri-net-based workflow tools.

Koschmider, A. and H.A. Reijers, 2015: Improving the process of process modelling by the use of domain process patterns; Enterprise Information Systems, v.9, no.1, p.29–57.

Abstract:

> The use of business process models has become prevalent in a wide area of enterprise applications. But while their popularity is expanding, concerns are growing with respect to their proper creation and maintenance. An obvious way to boost the efficiency of creating high-quality business process models would be to reuse relevant parts of existing models. At this

point, however, limited support exists to guide process modellers towards the usage of appropriate model content. In this paper, a set of content-oriented patterns is presented, which is extracted from a large set of process models from the order management and manufacturing production domains. The patterns are derived using a newly proposed set of algorithms, which are being discussed in this paper. The authors demonstrate how such Domain Process Patterns, in combination with information on their historic usage, can support process modellers in generating new models. To support the wider dissemination and development of Domain Process Patterns within and beyond the studied domains, an accompanying website has been set up.

Panchal, J.H., S.R. Kalidindi, and D.L. McDowell, 2013: Key computational modeling issues in integrated computational materials engineering; Computer-Aided Design, v.45, no.1, p.4–25.

Abstract:

Designing materials for targeted performance requirements as required in Integrated Computational Materials Engineering (ICME) demands a combined strategy of bottom–up and top–down modeling and simulation which treats various levels of hierarchical material structure as a mathematical representation, with infusion of systems engineering and informatics to deal with differing model degrees of freedom and uncertainty. Moreover, with time, the classical materials selection approach is becoming generalized to address concurrent design of microstructure or meso structure to satisfy product-level performance requirements. Computational materials science and multi-scale mechanics models play key roles in evaluating performance metrics necessary to support materials design. The interplay of systems-based design of materials with multi-scale modeling methodologies is at the core of materials design. In high performance alloys and composite materials, maximum performance is often achieved within a relatively narrow window of process path and resulting microstructures.

Much of the attention to ICME in the materials community has focussed on the role of generating and representing data, including methods for characterization and digital representation of microstructure, as well as databases and model integration. On the other hand, the computational mechanics of materials and multidisciplinary design optimization communities are grappling with many fundamental issues related to stochasticity of processes and uncertainty of data, models, and multiscale modeling chains in decision-based design. This paper explores computational and information aspects of design of materials with hierarchical microstructures and identifies key underdeveloped elements essential to supporting ICME. One of the messages of this overview paper is that ICME is not simply an assemblage of existing tools, for such tools do not have natural interfaces to material structure nor are they framed in a way that quantifies sources of uncertainty and manages uncertainty in representing physical phenomena to support decision-based design.

2 EARTH SYSTEM MODELLING: STATE OF THE ART AND LESSONS

Unlike all approaches presented in the first section, earth system modelling is normally performed in highly specialized modelling agencies. These agencies generally deal with large-scale, computation-intensive and high-complexity models that are of high practical significance, such as coastal current models that support marine navigation, weather forecast models that provide predictions, or climate change models. The high conceptual complexity, computational sophistication, and need for quality control has required differentiation of modelling tasks (research, observation, data management, model software development, model experimentation, hardware handling, quality control, training, communication, etc.).

A recent book series reviews how these agencies bridge the gap between information technology (IT) solutions and science, and provides important lessons for the other hydrological disciplines that are becoming increasingly computation-intensive.

2.1 Earth System Modelling Series – An Overview

Many of the literature-gleaned insights on large-scale, computation-intensive and high complexity models are summarized in a series on ''Earth System Modelling''. This series aims at bridging the gap between IT solutions and earth system science. Earth system models are conceptually assembled in a hierarchy of submodels, where process models are linked together to form one component of the earth system (e.g., atmosphere and ocean), and these components are then coupled together to earth system models in different levels of completeness. The software packages of the many process models usually comprise many thousand lines of code, which results in a high level of complexity to develop, optimize, maintain, and apply these assembled packages.

Running these models is an expensive business because they can only be executed on high-performance computers and often take months to conclude. This makes it highly attractive to increase the efficiency of the codes. Because the lifetime of the codes exceeds the typical lifetime of computing systems and architectures this requires that the codes be portable and adaptable to emerging computing technology. Although reductions in model runtimes was, in the past, achieved mainly from increasing clock speeds of the CPUs, today, processor speeds have apparently reached their limit. Therefore, current avenues for increased model performance speed can only be gained through innovative programming and code parallelism.

All of these requirements put high demands on programmers to apply software development techniques to the codes to make them readable, flexible, well structured, portable, and reusable. Fortunately, code development from many research centres has similar requirements in that it has to be done by scientific experts who typically are not computing or software development experts. Quality control, carried out by staff with detailed knowledge and experience in scientific software development that bridges computing and science, is necessary to assure fulfilment of the above.

Common software infrastructures or frameworks are an increasingly important in ensuring high model quality since they provide certain standards in terms of coding and interfaces, as wells as data formats and source management structures, and therefore enable code developers to solve problems more efficiently. Common frameworks foster: i) the exchange of codes between research institutions; ii) model inter-comparison projects that are valuable for model development; and iii) flexibility to the scientists when moving from one institution to another.

The topics covered in the series provide insight into state-of-the-art software solutions and in particular address: i) the coupling of software and strategies in regional and global models; ii) the coupling of infrastructure with data management; iii) strategies and tools for pre- and post-processing; and iv) techniques to improve the model performance.

Puri, K., R. Redler, and R. Budich, 2013: Earth System Modelling – Volume 1: Recent Developments and Projects; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3—642-36597-3

Summary:

This volume addresses the usefulness of coupling infrastructures and data management, strategies and tools for pre- and post-processing, and coupling software and strategies in regional and global coupled climate models. This first part in the series of 6 books sets the scene for the following volumes, and describes several ongoing projects.

Bonaventura, L., R. Redler, and R. Budich, 2013: Earth System Modelling – Volume 2: Algorithms, Code Infrastructure and Optimisation; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3-642-23831-4

Summary:

This volume addresses the historical development, state of the art and future perspectives of the mathematical techniques employed for numerical approximation of the equations describing atmospheric and oceanic motion. Furthermore, it describes the main computer science and software engineering strategies employed to turn these mathematical methods into effective tools for understanding earth's climate and for forecasting its evolution. These methods and the resulting computer algorithms lie at the core of earth system models and are essential for their effectiveness and predictive skill.

Chapters include:

- Numerical Algorithms for ESM: State of the Art
- Numerical Algorithms for ESM: Future Perspectives for Atmospheric Modelling
- Numerical Algorithms for ESM: Future Perspectives for Ocean Modelling
- Efficiency for Adaptive Triangular Meshes: Key Issues of Future Approaches
- Code Design and Quality Control
- Code Optimisation
- Code Parallelisation On Massively Parallel Machines
- Future Perspectives

Valcke, S., R. Redler, and R. Budich, 2012: Earth System Modelling – Volume 3: Coupling Software and Strategies; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3-642-23360-9

Summary:

This volume addresses the major coupling software developed and used in the climate modelling community.

Chapters include:

- TDT: A Library for Typed Data Transfer
- The Model Coupling Toolkit
- The OASIS Coupler
- The Flexible Modeling System
- The Earth System Modeling Framework
- The Bespoke Framework Generator
- Future Perspectives

Balaji, V., R. Redler, and R. Budich, 2013: Earth System Modelling –Volume 4: IO and Postprocessing; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3-642-36464-8

Summary:

This volume addresses the issue of data input/output (IO) and post-processing in the context of earth system modeling, with an emphasis on parallel I/O, storage management and analysis subsystems for very large scale data requirements.

Chapters include:

- Parallel I/O Basics
- ESM I/O Layers
- Data Storage
- Data Representation
- Data Analysis and Visualization
- Future Perspectives

Ford, R., G. Riley, R. Budich, and R. Redler, 2013: Earth System Modelling - Volume 5: Tools for Configuring, Building and Running Models; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3-642-23932-8

Summary:

This book is concerned with the source code version control of code components, the configuration of these components into earth system models, the creation of executable(s) from the component source code and related libraries and the running and monitoring of the resultant executables on the available hardware.

Chapters include:

- ESM Workflow
- Applying Scientific Workflow to ESM
- Configuration Management and Version Control in Earth System Modelling
- Building Earth System Models
- Running and Monitoring

- Configuring, Building and Running Models in GENIE
- Configuring, Building and Running Models in CIAS
- Summary and Conclusions

Hiller, W., R. Budich, and R. Redler, 2013: Earth System Modelling – Volume 6: ESM Data Archives in the Times of the Grid; Springer-Verlag, Berlin Heidelberg, Germany, DOI 10.1007/978-3-642-37244-5

Summary:

This volume addresses the Grid software which has become an important enabling technology for several national climate community Grids that led to a new dimension of distributed data access and pre- and post-processing capabilities worldwide.

Chapters include:

- Distributed Archives, Databases and Data Portals: The Scene
- Harvesting of Metadata with Open Access Tools
- Data Discovery: Identifying, Searching and Finding Data
- User Driven Data Access Mechanisms
- Collaborative Climate Community Data and Processing Grid—C3Grid: Workflows for Data Selection, Pre- and Post-Processing in a Distributed Environment
- Earth System Grid Federation: Federated and Integrated Climate Data from Multiple Sources
- Future Perspectives

APPENDIX 3

SAMPLE AGREEMENTS

SHARING AGREEMENTS

The following agreements have been amended from those used in the Oak Ridges Moraine Groundwater Program (ORMGP). In certain cases there might be a desire for consultants to make use of certain elements of a numerical model rather than the model itself. The data and information sharing agreement can serve in such cases. It should be noted that the following agreements are likely to evolve as they are put into practice. The most up-to-date forms can be found on the ORMGP's website (http://www.oakridgeswater.ca).

Data and Information Sharing Agreement

This Agreement dated this ____________ day of _________________, 20___

Between:

____ ***(Data "Owner")***

And

____ ***(Data "User")***

SECTION A: DATA AND/OR INFORMATION REQUESTED

"User" *TO INSERT THE TEXT OF THE REQUEST HERE (PROVIDE A SHORT DESCRIPTION OF THE DATA AND/OR INFORMATION REQUESTED AND, IF HELPFUL, ATTACH THE REQUEST FOR DATA AND/OR INFORMATION AS AN APPENDIX TO THIS AGREEMENT.)*

SECTION B: PURPOSE FOR THE DATA AND/OR INFORMATION REQUESTED

"User" *TO DESCRIBE THE PROJECT OR STUDY FOR WHICH THE REQUEST IS BEING MADE.*

SECTION C: DISCLAIMER

The following disclaimer applies to the disclosure of the Data and/or Information requested. While efforts are made to ensure that the Data and/or Information supplied in response to the request is accurate and up to date:

i) neither the ***"Owner"*** nor any of their employees or officers shall be liable for any damages, or suffer any loss arising from any errors or inaccuracies therein, or from any misuse, misinterpretation or misapplication thereof by the ***"User"***, whether due to the negligence, omission, or activities of such employees or officers or otherwise; and

ii) the said Data and/or Information is made available to the ***"User"*** solely on condition that the ***"User"*** and the ***"User's"*** heirs, executors, administrators, successors and assigns assume full responsibility for any risk associated with the use or misuse thereof, and agree to indemnify and hold harmless the ***"Owner"*** and their employees, appointed officials and officers from any and all damages or losses whether arising directly or indirectly from the disclosure of the data and information, including all damages and losses of the type described in clause (i) above.

SECTION D: CONDITIONS

The following conditions apply to the release of Data and Information:

i) The ***"Owner"*** must be acknowledged as the agency from which the Data and/or Information was obtained in any reports prepared by the ***"User"*** for any person, or in any publications of any kind;

ii) The ***"User"*** will bring to the attention of the ***"Owner"*** any errors detected in the Data and/or Information;

iii) The Data and/or Information described in Section A will be used exclusively for the purpose described in Section B and any other use of the Data and/or Information shall be subject to the written permission of the ***"Owner"***;

iv) The ***"User"*** will not disclose, in digital or any other form, the Data and/or Information to third parties without the explicit written permission of the ***"Owner"***;

v) The ***"Owner"*** hereby gives the ***"User"*** explicit written permission to share the Data and/or Information, as required, with the Ministry of the Environment and Climate Change of the Province of Ontario or its successor ministry;

vi) The ***"User"*** shall supply back to the ***"Owner"*** any Data and/or Information acquired during the course of the project to meet the needs for the purpose described in Section B and provided in a digitized format;

vii) The ***"User"*** acknowledges and agrees that the collection, use and disclosure of the Data and/or Information provided by the ***"Owner"*** shall be governed by the provisions of the *Municipal Freedom of Information and Protection of Privacy Act*, R.S.O. c. M.56, as amended, including but not limited to section 10 thereof;

viii) The Data and/or Information will remain the property of the ***"Owner"*** and all intellectual property rights in such Data and/or Information remain vested in the ***"Owner"***; and

ix) In the event the ***"User"*** undergoes a change in either ownership or organization, this agreement will become null and void and all Data and/or Information provided shall be immediately returned to the ***"Owner."***

I ACKNOWLEDGE AND AGREE TO THE ABOVE DISCLAIMER AND CONDITIONS:

NAME: ______________________________ POSITION: __________________

FIRM: ____

SIGNATURE: _________________________ DATE: ____________________

As Witnessed By:

NAME: ______________________________ POSITION: __________________

FIRM: ____

SIGNATURE: _________________________ DATE: ____________________

Numerical Model Sharing Agreement

This Agreement dated this ____________ day of _________________, 20___

Between:

____ ***("Owner")***

And

____ ***("User")***

For the request of

____ ***("Model Name")***

To fulfill the requirements of

____ ***("Project Name")***

SECTION A: DEFINITIONS

For this Numerical Model Sharing Agreement, the following terms will be used:

"Owner" refers to the agency (or partnership of agencies/consulting companies) that has ownership of the numerical model.

"User" refers to individuals/firms/agencies that are seeking to make use of the numerical model.

"Model" refers to the numerical model hereinafter referred to as the ***"Model Name"***, as requested by the ***"User"*** and provided by the ***"Owner"*** under the terms of this model sharing agreement. The term ***"Model"*** is implicit in reference to all elements of the numerical model required in reproducing model results, including:

i) The model executable(s) and model code version number(s);

ii) Data used to construct (i.e., model structural files, model parameters) and to run the model (input variables) for any variant (e.g., scenario) of the model used in production of model results; and,

iii) All model control files that are required to run any model variant (e.g., calibration, validation, baseline, scenario, etc.).

The ***"Owner"*** will assign a ***"Model Name"*** as a reference to the provided ***"Model"*** to which the ***"User"*** must adhere to when reporting on the ***"Model"*** provided. Unless specifically requested by the ***"Owner"***, the use of the ***"Model Name"*** is restricted from being used in reference to any models produced by the ***"User"*** as a ***"Derivative"***.

"Project Name" refers to the name of the project for which the ***"User"*** wishes to make use of the ***"Model"***.

"Derivative" refers to any model produced by the ***"User"*** that was in any way informed, founded upon or based on the provided ***"Model"***. ***"Derivative"*** includes any model utilized by the ***"User"*** in which the ***"Model"*** structure changes (e.g., local refinements, parameter changes, boundary condition changes, etc.) have been made to fulfill the needs of the ***"Project Name"***.

SECTION B: MODEL(S) REQUESTED

"User" *TO INSERT THE TEXT OF THE REQUEST HERE (PROVIDE A SHORT DESCRIPTION OF THE MODEL BEING REQUESTED AND, IF HELPFUL, ATTACH THE REQUEST FOR DATA AND/OR INFORMATION AS AN APPENDIX TO THIS AGREEMENT.)*

SECTION C: INTENDED USE OF THE REQUESTED MODEL(S)

"User" *TO DESCRIBE THE PROJECT OR STUDY FOR WHICH THE REQUEST IS BEING MADE AND THE INTENTIONS OF THE MODEL (E.G., RESULTS TO BE GAINED, REFINEMENTS EXPECTED TO BE MADE, ETC.).*

SECTION D: BACKGROUND CONTEXT TO AGREEMENT

This agreement has been prepared in the spirit of improving water management decision making in the Province of Ontario. The ***"Owner"*** is intending to actively maintain the ***"Model Name"*** into the future. Long term active model maintenance includes keeping an up-to-date database upon which the model is based, as well as incorporating into the ***"Model Name "*** new insights and/or interpretations that arise as various users work with the model. Upon each new use of the model, the ***"Owner"*** requests that a new agreement be signed to allow for the ***"Model Name"*** to be kept up to date and that the most recent data, analyses and interpretations can be brought to bear on each new study.

SECTION E: NUMERICAL MODEL DISCLAIMER/LIMITED WARRANTY[1]

The ***"Owner"*** does not warrant the ***"Model Name"*** or any associated software to be correct, free from defects, suitable for any purpose, or compatible with any model of computer.

Because the model is inherently complex, it is the responsibility of the ***"User"*** to verify the model or any associated software and any work produced using these. The ***"Owner"*** rejects all liability and responsibility relating to the consequences of using the ***"Model Name"*** and its ***"Derivatives"***. In no event will the ***"Owner"*** be liable for indirect, incidental, economic or consequential damages arising out of the use of the model, including, without limitation, damages or costs relating to loss of revenue or profits, business, goodwill, data or computer programs, or claims by a third party. Except for representations and warranties expressly made in this Agreement, the model is provided on an "as is"

[1] This Disclaimer/Limited Warranty has been adapted from a waiver available at the National Research Council of Canada's website (http://www.nrc-cnrc.gc.ca/eng/solutions/advisory/blue_kenue/terms.html [accessed 2016]). It provides a reasonable template which can be adjusted to suit the needs of government agencies that wish to share numerical models with external unaffiliated parties.

basis, and there are no representations or warranties, express or implied by statute, including, without limitation, any with respect to:

i) Merchantability or fitness for any purpose.

ii) Operational state, character, quality or freedom from defects.

The ***"User"*** shall indemnify and save harmless the ***"Owner"***, their employees and agents from and against, and be responsible for:

i) All claims, demands, losses, damages, costs including solicitor and client costs, actions, suits or proceedings brought by any third party, that are in any manner based upon, arising out of, related to, occasioned by, or attributable to the use of the ***"Model Name"*** and its ***"Derivatives"***.

ii) Other costs, including extra-judicial costs, of the ***"Owner"*** defending any such action or proceeding, which the ***"Owner"*** shall have the right to defend with counsel of their choice.

SECTION F: AGREEMENT

This agreement between the ***"Owner"*** and ***"User"*** allows for the use of the ***"Model Name"***. The ***"Owner"*** is allowing access of the ***"Model Name"*** to the ***"User"*** for the sole purpose of the ***"Project Name"*** at no charge in the interests of promoting sound water management decision making. As a result, the use of the ***"Model Name"*** is subject to the following conditions:

1) The ***"Model Name"*** and any ***"Derivatives"*** can only be used by the ***"User"*** exclusively to fulfil the purposes of the ***"Project Name"*** as outlined in Section C.

2) Regardless of how significantly the ***"Model Name"*** might change as a result of work undertaken on the "***Project Name"*** the ***"Owner"*** still retains ownership of the ***"Model Name"***.

3) Upon completion of the "***Project Name"***, the ***"User"*** agrees to return the ***"Model Name"*** and any ***"Derivatives"*** to the ***"Owner"*** as used to fulfil the purposes of the ***"Project Name"*** as outlined in Section C. The purpose of this request is to provide the ***"Owner"*** with the opportunity to update the ***"Model Name"*** with any new data, insights, and understanding that may have been incorporated into a ***"Derivative"*** as a result of the "***Project Name"***.

4) Upon completion of the "***Project Name"***, and at the specific request of the ***"Owner"***, the ***"User"*** (along with their technical modelling sub-consultants, if applicable) agrees to attend a technical meeting with the ***"Owner"*** in order to convey to agency staff any new data, insights and understandings that have been incorporated into any ***"Derivative"*** as a result of the "***Project Name"***. The ***"User"*** staff time costs for the meeting are to be borne by the ***"User"***.

5) Unless specifically requested by the ***"Owner"***, and regardless of whether the ***"Model Name"*** is used as provided and no ***"Derivative"*** is produced, the ***"User"*** agrees that any documentation prepared for the "***Project Name"*** must not use the term ***"Model Name"*** without adding a prefix, suffix, modifier or qualifier, or changing the model name altogether, to convey that that the results are not part of the original intention of the ***"Model Name"***. Reference must still be given

to the ***"Model Name"*** in all documentation, as it nonetheless formed the basis for the analyses undertaken for the "***Project Name"***.

6) The ***"Owner"*** assumes no liability whatsoever for any decisions that may arise as a result of the ***"User"*** having made use of the ***"Model Name"*** and any ***"Derivative"*** for the purposes of the ***"Project Name"***.

7) This agreement is effective from the date of signature (below) until the ***"Owner"*** has received back the ***"Model Name"*** and any ***"Derivative"*** from the ***"User".***

I ACKNOWLEDGE AND AGREE TO THE ABOVE DISCLAIMER AND CONDITIONS:

NAME: ____________________________ POSITION: _________________

FIRM: ____

SIGNATURE: _______________________ DATE: ___________________

As Witnessed By:

NAME: ____________________________ POSITION: _________________

FIRM: ____

SIGNATURE: _______________________ DATE: ___________________

REQUEST FOR PROPOSAL DOCUMENT EXAMPLES

The following section builds upon what is presented in Section 5.3 in the main body of this guidance manual and provides a set of example clauses that agencies can add into, or build upon, when drafting Request for Proposals (RFPs) for new modelling studies. Of course, anything presented below can be altered or tailored to meet the needs of any public sector agency. Section 5.3 describes five necessities that should be incorporated into any RFP. All are somewhat addressed in the samples below, they include:

i) project expectations;
ii) data expectations;
iii) expected deliverables;
iv) model reporting requirements; and
v) declaration of intellectual property rights.

The first part of this appendix provides sample sharing agreements with clauses and descriptions that the reader is free to use for RFP development. Data delivery expectations followed by a generic yet all-inclusive list of expected deliverables follows. These can also be copied and altered where necessary for use in RFP documents. The example delivery list provided below is intentionally descriptive, since experience has shown it to be necessary for ensuring complete model file delivery. Lastly, within the main body of the manual, detailed discussions can be found on reporting requirements (Section 5.3.4 and 5.7.2) and on intellectual property rights (Sections 4.2 and 5.3.5).

Project Description and Future Use Clauses

The RFP should ensure up front that all consultants bidding on a model project are aware that the model is to be used for the immediate needs of the agency in solving the current water resources challenge, and that the model may also be used for the agency's long-term water resources management plans.

Sample 1

> Although this modelling project is being driven by the current need to help with resolving water issues in the vicinity of ***Project Name***, the ***Agency Name*** is also interested in the use of a numerical model for providing assistance with longer term water resources management within a broader context. Possible uses of the model into the future include: i) assessment of development proposals on both groundwater and surface water resources; ii) assessing proposed surface water diversions/takings; iii) assessing groundwater pumping proposals; iv) delineating important hydrological areas that might require additional policies within the Official Plan; and v) assessing potential impacts to ecological features, etc.

Sample 2

> Given the above, consultants are explicitly informed (and agree) that the ***Agency Name*** may at any point in the future turn over the model files prepared under this agreement to other consulting firms working for the ***Agency Name***, as a starting off point for other, as yet unknown, miscellaneous hydrological and/or hydrogeological projects. Proposals should explicitly state

that the consulting company has no reservations with the ***Agency Name*** sharing model files with other consultants and/or agencies subsequent to the completion of the project.

Sample 3

The ***Agency Name*** is intending to not only use the model to […*ADD RELEVANT DETAILS HERE*…], but in the longer term, also intends to update and use the model as an ongoing tool for staff to […*ADD RELEVANT DETAILS HERE*…]. In addition, there is the possibility that the model could also be used as a starting off point (i.e., it can be altered as necessary) by other consultants working for the ***Agency Name*** on other, as of yet unknown, miscellaneous hydrological, hydrogeological, and/or […*ADD RELEVANT NEEDS HERE*…] evaluations.

Intellectual Property Rights (Model Results) Clauses

Given the potential for the **Agency Name** to make use of the model for longer term water management, the RFP should explicitly address intellectual property/model ownership.

Sample 1

The ***Agency Name*** may be interested in using the model prepared under this RFP for longer term water resources management. As such, the ***Agency Name*** will require the transfer of all files needed in order to run the model to completion. The ***Agency Name*** intends to become the sole owner of the proposed numerical model and has the right to determine: i) whether a numerical model is used for any given project; and ii) who (i.e., which agencies/individuals) are permitted to make use of the model. As such, the ***Agency Name*** is interested in retaining a consulting firm that is willing to transfer to the ***Agency Name*** model ownership/intellectual property rights at the conclusion of the project. The consultant agrees that the prepared model will be exclusively owned by the ***Agency Name*** and that the consultant will have no right to use the model for any other project unless a written request has been submitted to the ***Agency Name*** and permission has been granted by the ***Agency Name*** in writing.

Should the consultant wish to propose an alternate ownership/intellectual property rights framework, they are encouraged to discuss this with the ***Agency Name*** staff prior to preparing their proposal, to ensure that their approach is satisfactory.

In order for the ***Agency Name*** to acquire the necessary software for future use of the model, submitted proposals must state which modelling software will be used to generate the model output results. If appropriate, any software programs, routines and/or scripts that will also be needed to reproduce model outputs should also be identified in the proposal.

Sample 2

As part of the project, the consultant agrees that the prepared model will be exclusively owned by the ***Agency Name***. In order for the consultant to use the model for any other project they will need to submit a written request to the ***Agency Name*** and receive permission from the ***Agency Name*** in writing.

Within the contract document, the consultant will agree to transfer intellectual property rights (IPR) to any data generated through the project to the ***Agency Name***.

Should the consultant wish to propose an alternate ownership/IPR framework, they are encouraged to discuss this with the ***Agency Name*** staff prior to preparing their proposal, to ensure that their approach is satisfactory.

Intellectual Property Rights (Proprietary Software, Workflow Scripts and Code Modifications) Clauses

Given the potential for the model to be used for the longer term, the RFP should explicitly address the issue of modified model software code and proprietary scripts.

Sample 1

The ***Agency Name*** is interested in potentially making use of the model for longer term water resources management decisions. As such, it is important for the ***Agency Name*** be able to make use of software codes to rerun the model into the future. For this reason, any code modifications to commercially available software are discouraged. If code modifications are to be used by your firm, they must be clearly disclosed within the proposal, along with the reasons for, and the advantages of, such code modifications. The ***Agency Name*** may request that the code modifications be made available up front for peer review and verification. Should the consultant be successful in being awarded the contract, at the conclusion of the project they will be required to transfer the modified code to the ***Agency Name***, and they agree that the ***Agency Name*** will be entitled to make use of the modified code for other projects. The code, along with the modelling files, will be used to ensure that the model reproduces the results documented in the final project report. The author, date, and details of the modifications must be indicated within the model delivery and described within the final project report.

In a similar manner, should your firm employ any pre- or post-modelling software programs and/or scripts to build, convert, translate, analyse, assemble, or interpolate model input files or to process model output files (e.g., for generating results, visualisations, tables, perform statistical analyses, model evaluation, etc.) then these must be disclosed, along with the reasons for their application, within the proposal. If such routines are not commercially available (i.e., written by your consulting firm), then the cost to acquire such software routines plus annual support fees must be disclosed within the proposal. If the scripts and/or software routines are necessary to reproduce the results then they must be made available to the ***Agency Name*** at the conclusion of the project and they may be distributed to other consultants or agencies working on future projects.

Sample 2

Within the proposal, the consultant must disclose the proposed software modelling code and version to be employed for the project as well as directions as to how the ***Agency Name*** can access this software and/or code for review, verification, and reproduction of results when necessary. If there are any known or proposed alterations to the model code that the consultant employs, they must be disclosed within their proposal along with a justification for their use and a discussion on how they improve upon the original code. At the completion of the project, the final model development report must incorporate general information regarding the modifications made (e.g., the author, date, and description of the modifications, and the reason behind their use). Where an alteration to pre-existing model code has been employed, a fully functional code must be delivered to the ***Agency Name*** at the completion of the project. The code, along with the modelling files, will be used to ensure that the model reproduces the results documented in the modelling report. The ***Agency Name*** will be entitled to make use of such coding for other projects. Consultants are hereby given notice that should the ***Agency Name*** retain a different consultant to make use of the model in the future for other projects, then the modified code and description would be passed on as part of the modelling package to the new consultant.

In cases where code modifications were made and/or scripts were employed for the sole purpose of improving the consultant's workflow, but in no way affects the numerical procedures within the model (i.e., does not have an effect on the model results), then the model should be delivered in a form that is completely compatible with the non-modified version of the model code.

Sample 3

Within the proposal, the consultant shall outline additional tools that are essential for reviewing, reproducing, updating, and legally defending the study results. These include tools and/or scripts for the conversion and analysis of raw data into input data; tools and/or scripts for configuring, building and running the models; and tools and/or scripts for evaluating model output data in order to generate results. The proposal shall list the role that the software plays for generating modelling results from raw data, specifying the type of software, the purpose for which it is used, associated intellectual property rights, available documentation, and accessibility options including licensing.

At the completion of the project, software tools and scripts, as outlined above, are to be handed over to the ***Agency Name*** should they be required in reproducing the reported results. The ***Agency Name*** would be entitled to make use of such coding in future uses of the model. Consultants are hereby given notice that should the ***Agency Name*,** in the future, retain a different consultant to make use of the model for other projects, then these scripts would be passed on as part of the modelling package to the new consultant.

Data Expectations Clauses

The RFP should include a section that clearly discusses the link between long-term modelling and the requirement for ready access to high quality water resources–related data.

Sample 1

Consultants are hereby notified that water resources–related data management is a key priority for the ***Agency Name***. The ***Agency Name*** is looking at this modelling project as an opportunity to enhance and build upon the ***Agency Name***'s existing data management program. At the onset of the current modelling project, the consultant will be provided with an up-to-date database. It is expected that over the course of the project that the consultant will add newly acquired data into the database (reflecting the format that is currently in use). The updated database is expected to be returned at the completion of the modelling project. New data as well as improvements to existing data will be re-incorporated into the ***Agency Name***'s master database. The ***Agency Name*** expects the final report to have a separate section that comments on the quality and breadth of the database provided at the onset of the project and also highlights key aspects of the database that may have been changed or supplemented over the course of the project.

Within their proposals, consultants are requested to explicitly comment on experience in managing data and their approach to implementing best practices in terms of data management. Data management costs should be provided for as a separate line item within the budget.

Sample 2

Inherent in the development of the requested model is the need for access to high quality data. The ***Agency Name*** is looking at this modelling project as an opportunity to enhance and build upon the ***Agency Name's*** existing data management program. To complete the current modelling project, the consultant will be provided with an up-to-date database. It is expected that over the course of the modelling project the consultant will add newly acquired data into the database (consistent with the database schema already in use). The updated database is to be returned at the completion of the modelling project. New data as well as improvements to existing data will be re-incorporated into the ***Agency Name's*** master database.

Model File Transfer Clauses

The RFP should address the transfer of modelling files at the conclusion of the project. As a full-proof means of assuring a complete model file transfer, it is strongly recommended that the project not be deemed complete until the model has been successfully run to completion on a local agency workstation.

Sample 1

Proposals should provide a section that discusses the transfer of modelling files to the ***Agency Name*** servers. File transfer costs must be clearly earmarked within the proposal and are expected to be associated with: i) portable hard disk drives (or other storage media), particularly if files sizes are expected to be large; and ii) consultant staff time necessary to transfer the files and ensure that the model can be run to completion on an ***Agency Name*** workstation. Note: the project will not be deemed finalized until the model has been successfully run to completion on the ***Agency Name*** computers. All transferred files must be delivered in the directory structure outlined below.

Sample 2

> Given that the model is to be used for the longer term at the ***Agency Name***, it is required that the consultant incorporate (and clearly separate) cost estimates into their proposal to transfer all model files to the ***Agency Name*** computers. Costs should not only be tied to the consultant time needed to properly transfer files, but in addition, if file sizes are anticipated to be very large, the cost of storage media must also be incorporated. All transferred files should come in the directory structure outlined below. The project will not be deemed to have been completed until the model has been successfully run to completion on an ***Agency Name*** workstation.

Communication Clauses

Some of the most successful modelling projects are often those where consultants and agency staff work together to understand the flow system and how the model is built to reflect the system. By working cooperatively both parties better understand the limitations and the power of the model in addressing overall water management needs. This type of knowledge transfer is an important consideration in commissioning modelling studies.

Sample 1

> Consultants are requested to outline their abilities and attitudes with respect to transferring modelling knowledge to the ***Agency Name*** staff. Knowledge transfer to the ***Agency Name*** staff, including your firm's overall approach to data management, technical communication skills, accessibility to modelling software, data processing scripts, as well as any other aspects will be considered when reviewing proposals.

Sample 2

> An approach to knowledge transfer, including the approach to data management, access to modelling software, data processing scripts, the overall architecture of software tools, and other aspects related to knowledge transfer to the ***Agency Name*** will be considered when assessing proposals.

Model Custodianship Clauses

Some agencies might not have strong information technology capabilities. For this reason, or for a number of other similar reasons, the RFP might incorporate longer term model file storage within the scope of the project. This can help guard against modelling files being misplaced, corrupted, or lost at the public sector agency offices.

Sample 1

> Consultants are requested to provide a cost for the long term (five year) storage of all files related to the model. Should the ***Agency Name*** agree to this cost, if the files at the ***Agency Name*** become corrupted, misplaced, or lost, the consultant would be expected to provide a full back-up of the final model files within a one-week period of such a request with only a minimal administrative cost being incurred.

Sample 2

> The consultant will provide a cost for the long term (five year) storage of all files related to the model. Should the files at the ***Agency Name*** become corrupted, misplaced, or lost, the consultant would be expected to provide a full back-up of the final model files within a one-week period of such a request with only a minimal administrative cost being incurred.

Data Delivery Requirements

Below is a list of common model files that should be requested to fulfill model delivery expectations. Again, in addition to the deliverables, it is strongly recommended that the project not be deemed complete until the model has been successfully run to completion on a local agency workstation.

Model reporting deliverables:

- All intermediate and final reports (draft reports not necessary).
- Technical documentation that is not included in the reports but is required to reproduce results, including descriptions on
    - how tables, figures, and maps were created, and
    - modelling workflows and software tools utilized.
- All shapefiles and rasters used in creating maps.
- All tabular data used in reports. These should be provided in a clear and intuitive form. If delivered in the form of Microsoft® Excel® files, the files must remain unlinked to other Excel files. It must be made clear as to the linkage between the table numbers in the report and the associated digital tables being delivered.
- If scripts and/or third-party software have been used to develop tables and figures from model outputs, a complete description of the scripts and/or software must be included.

Model files deliverables:

- All digital project files [… ENTER APPRORIATE PROJECT PLATFORM IF KNOWN, e.g., ArcGIS, QGIS, Manifold, FEFLOW, Viewlog, Visual MODFLOW, GMS, Groundwater Vistas, ETC.…] used in building the model structure, preparing model input files and/or producing report figures must be provided at the conclusion of the project. All project files must be delivered, installed, and in full working-order on the **Agency Name** workstations.
- Graphical software project files (e.g., MatLab, R, Microsoft Excel, Golden Grapher/Surfer, TecPlot, ParaView, etc.) used in creating any report tables, charts, and figures must be provided at the conclusion of the project.
- [… *FOR GROUNDWATER MODELLING ONLY* …] The 3D conceptual model files used to represent interpolated units and their hydraulic properties (i.e., hydraulic conductivity, storage coefficient, specific yield, porosity, layer thickness, tops and bottoms, vertical conductance or anisotropy ratios, etc.) must be provided at the conclusion of the project in standard geospatial raster format – either in ASCII-format (*.asc;*.xyz) or binary format (*.flt). Files must be appropriately and intuitively labelled according to the property they represent and the

geological/hydrogeological unit they refer to. Files must be provided regardless of whether the conceptual model was built using a proprietary model-building software tool.

- Shapefiles and/or rasters used in defining any feature/boundary conditions used in building the numerical model (e.g., digital elevation model, waterbodies, watercourses, land use, pits and quarries, soils classification, surficial geology, land use classification, hydraulic structures, etc., and/or any other spatial structure used in model design), fully attributed with the parameterisation they impose on the model or indices used to join the shapefile/raster to a parameter lookup table, must be provided at the conclusion of the project.
- The digital elevation model used in defining the model grid/mesh and a description of its source must be provided at the conclusion of the project. If a finite-difference grid is employed, then digital elevation must be resampled to the grid definition to match the model structure and provided in a standard format (*.asc;*.xyz). If a finite element or flexible mesh is employed, then the mesh must be delivered as two shapefiles (*.shp): a point shapefile attributed with finite element node IDs, and a polygon shapefile attributed with the finite element IDs.
- Database(s) that include all pumping information, surface water takings, geological interpretation (i.e., picks and constraining polylines), calibrations targets, etc., used in the construction, calibration, and evaluation of the model must be provided at the conclusion of the project.
- Model executable files, with model version/release clearly indicated, must be provided at the conclusion of the project.
- If code modifications are made and the official release of the modelling software is inadequate to run the numerical model using the input files provided, a detailed and complete explanation of the model version from which the modifications were made and a description of and rationale for the modifications must be provided along with the author and date of the modifications.
- Where internal numerical modelling processes have been directly modified, the modified source code must be provided and fully commented. Otherwise,
    - where only the input and output formats of the model are modified, then the model must be delivered in the standard model input file format, which can be readily run using the official release of the (unmodified) modelling code; and
    - any pre-processing scripts/routines required in building model input files and running the model and/or post-processing scripts required in producing model results specific to the requirements of this proposal must be provided at the conclusion of the project.
- Model input files (i.e., control, parameter, input variables) in an organized and intuitive file structure must be provided at the conclusion of the project. The files will be relocated and immediately run to completion on an ***Agency Name*** workstation. Model inputs for all reported runs (calibration, baseline, validations, scenario, etc.) must be included.
- All model output files for the baseline and/or calibration run only should be clearly identified and must be included to ensure that the model results are reproducible. Model output files must be provided at the conclusion of the project and must be immediately reproducible by the ***Agency Name*** after rerunning the delivered model.

- Baseline model output files must be delivered in a standard format. The 1D temporal data must be provided for each spatial location (either one file per location or a structured database format). Data columns should, at a minimum, include 'LOCATION, DATE, VALUE, UNITS, COMMENT,' where the comment field should include relevant information on data quality (e.g., whether it was measured or infilled, interpolated, etc.). The 2D temporal data must be provided in standard time-stamped raster data (e.g., NetCDF). The data delivery must include both model input and output data, regardless of whether the data are unmodified from the data received by the consultant at project start-up.
- If parameter estimation routines or uncertainty analysis was performed using a third party software (i.e., PEST, UCODE, OSTRICH, UNICORN, MICA, NLFIT, etc.) then control files used in conjunction with the model(s) must be included. If global sensitivity analysis or Monte Carlo sampling has been employed as part of an uncertainty analysis, then the full description of the methodology must be provided in the model report.

LEGAL AGREEMENT CLAUSES

The following are clauses that can be incorporated into a Legal Agreement between a consultant and a public sector agency to address key numerical modelling–related aspects of any particular project. Of course these can be adjusted to meet local agency needs and indeed other acceptable paths forward can be proposed by others, either consulting firms or public sector agencies. The clauses are adapted from previously reviewed contract documents and it is always recommended that the agency's legal counsel review and approve of any legal agreements.

Ownership of Model and Associated Files Clause

The ***Agency Name*** shall have the sole and exclusive title to the future use of the numerical model being constructed. This would include drawings, reports, data files, model files, specifications and any other documentation (both electronic and hard copy) prepared in connection with the Project. The Consultant shall be entitled to retain a copy of the numerical model and all documents and drawings produced for the Project but shall not disclose or release any modelling results, modelling files, drawings, documents, specifications, and any other documentation prepared in connection with the Project, or copies thereof, to any person or organization without the prior written consent of the ***Agency Name*** at any time before, during or after the completion of the Project.

Defining Intellectual Property Clause

For purposes of this Agreement, "Intellectual Property" means any intellectual, industrial or other proprietary right of any type in any form protected or protectable under the laws of Canada, any foreign country, or any political subdivision of any country, including, without limitation, any intellectual, industrial or proprietary rights protected or protectable by legislation, by common law or at equity.

Transfer of Intellectual Property Clause

> The ***Agency Name*** shall be the sole owner of any newly created Intellectual Property. The Consultant irrevocably assigns to and in favour of the ***Agency Name*** and the ***Agency Name*** accepts every right, title and interest in and to all newly created Intellectual Property in the deliverables, immediately following the creation thereof, for all time and irrevocably waives in favour of the ***Agency Name*** all rights of integrity and other moral rights to all newly created Intellectual Property in the deliverables, immediately following the creation thereof, for all time.

Addressing Consultant Intellectual Property Clause

> To the extent that any of the project deliverables include, in whole or in part, the Consultant's Intellectual Property, the Consultant grants to the ***Agency Name*** a licence to use that Consultant's Intellectual Property in the manner contemplated in this Article, the total consideration for which shall be payment of the rates to the Consultant by the ***Agency Name***.

Addressing Multiple Agencies Funding a Modelling Study Clause

In the case whereby funding is provided or contributed by one agency to another to oversee and carry out a modelling study (e.g., where a regional municipality funds a conservation authority or a local municipality to undertake a modelling study) or in cases where one agency enters into the agreement with the consultant but more than one agency has partnered or contributed funds for a modelling study and where partnered/contributing agencies wish to retain the rights to make use of the model into the future, the following clause can be used.

> ***Name of Lead Agency*** (receiving funding) hereby grants to the ***Name of Funding Agency*** a non-terminable, perpetual, royalty-free, non-exclusive, worldwide licence to use, distribute, reproduce, sublicense, manufacture, copy and otherwise deal with, for such purposes and uses as the ***Name of Funding Agency*** in its sole opinion, determines advisable or necessary, all reports, budgets, products, studies, compilations and collections of data, and other materials and documentation written, designed or produced by or for the ***Name of Lead Agency*** (receiving funding) to or in connection with this agreement in any medium or format (collectively, the project output) and in which the ***Name of Lead Agency*** (receiving funding) holds any Intellectual Property. The ***Name of Lead Agency*** (receiving funding) represents and warrants that it shall at all material times have the rights, title and/or interest in and to the Intellectual Property embodied in the project output that it needs to make this grant of licence to the ***Name of Funding Agency***. The above licence and warranty in this section, shall survive any termination, or expiry of this Agreement, and remain in full force and effect thereafter.