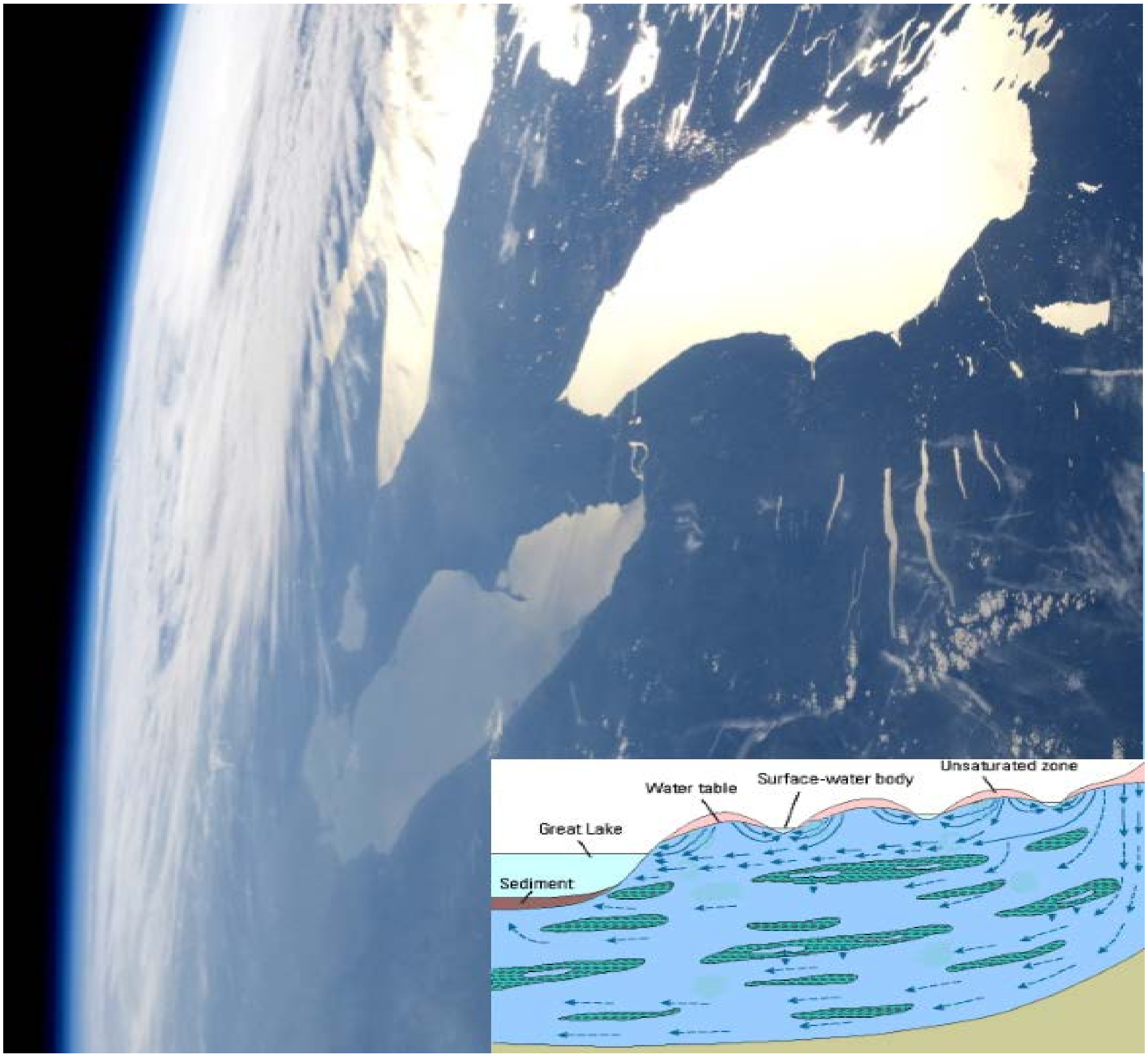
Great Lakes Surface and Groundwater Model Integration Review

Literature Review, Options for Approaches and Preliminary Action Plan for the Great Lakes Basin



Prepared by the
Great Lakes Science Advisory Board
Research Coordination Committee

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In the Great Lakes Region, Water Resources Investigations Report 00 – 4008, Figure 3

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Glossary of terms

Base flow provides a relatively stable supply of water, typically with high clarity and stable temperature. Base flow is alternatively termed indirect ground-water discharge by some authors. This streamflow is important to stream biota and helps support recreation-based industries (B P Neff et al. 2005). The term also is used as one word (baseflow) by some researchers.

MODFLOW-NWT is a standalone model developed by the United States Geological Survey (USGS); it is a Newton-Raphson formulation for MODFLOW-2005 to improve solution of unconfined groundwater-flow problems, in particular those involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation (Niswonger, Panday, and Ibaraki 2011).

Abbreviations

Abbreviation	**Meaning**
2D	Two dimensional
3D	Three dimensional
ACME	Accelerated Climate Modeling for Energy (United States DOE)
AHPS	Advanced Hydrologic Prediction System (NOAA)
AHPS	Advanced Hydrologic Prediction Service (National Water Model)
AFINCH	Analysis of flows in network channels (a surface water model)
CAMC	Conservation Authorities Moraine Coalition
DOE	Department of Energy (United States)
ECCC	Environment and Climate Change Canada
GEM	Global Environmental Multi-scale model
GLAHF	Great Lakes Aquatic Habitat Framework
GLERL	Great Lakes Environmental Research Laboratory, NOAA
GLHD	Great Lakes Hydrography Dataset
GRACE	Gravity Recovery and Climate Experiment
GW-SW	Groundwater - surface water
HGS	HydroGeoSphere (an integrated groundwater-surface water model)
IJC	International Joint Commission
INRS	Institut national de la recherche scientifique, Québec
IPCC	International Panel on Climate Change
LSM	Land surface model
MEC	Modélisation Environnementale communautaire (ECCC)
MECP	Ministry of the Environment, Conservation and Parks (Ontario), formerly MOECC
MNRF	Ministry of Natural Resources and Forestry (Ontario)
MOECC	Ministry of Environment and Climate Change (Ontario); Note the name of this ministry changed in June 2018 to MECP
MONDM	Ministry of Northern Development and Mines (Ontario)
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research (United States)
NEMO	Nucleus for European Modeling of the Ocean
NLDAS	North American Land Data Assimilation System
NRCan	Natural Resources Canada
NOAA	National Oceanic and Atmospheric Administration (United States)
NWM	National Water Model (United States)

PEST	Parameter ESTimation
SNTEMP	Stream-Network TEMPerature model
SVAT	Soil-vegetation atmospheric transfer
SWAT	Soil and Water Assessment Tool
TNC	The Nature Conservancy
USGS	United States Geological Survey
WCPS	Water Cycle Prediction System
WRF	Weather Research and Forecasting model (lead agency NCAR)

Executive summary

The International Joint Commission's Great Lakes Science Advisory Board has identified a need for a basin-scale assessment of the influence of groundwater on water quantity and quality of the Great Lakes basin. A first step in developing a basin-scale understanding is to develop a satisfactory model of the hydrologic contributions of groundwater to the water balance of the system. While there is some understanding of the contribution of groundwater to quantity and quality at regional scales, there is a gap at the basin scale.

Knowledge of groundwater's contribution to the water budget for the Great Lakes basin is needed, since both direct groundwater discharge (from rocks and glacial sediment to the lakebeds) and indirect discharge (to rivers and streams as base flow) have effects on water quality and quantity. For instance, contaminated groundwater from various land use activities can have a detrimental effect on potable water supplies, Great Lakes ecosystems and other water uses. Knowledge of groundwater flow regimes is critical from a water security perspective so sensitive aquifers can be protected from contamination. Understanding the water balance is also essential for better modeling of drought and flood conditions and for better predicting basin-scale hydrologic changes from changing climatic trends.

This report summarizes the results of a literature review, a survey of science experts, workshop discussions, and a resulting initial action plan to develop an integrated groundwater-surface water (GW-SW) model for the Great Lakes basin. The Great Lakes Science Advisory Board's Research Coordination Committee managed the initiative, with the assistance of a steering committee and a consulting team.

The literature review included government reports and peer-reviewed literature of relevant publications pertaining to groundwater modeling, surface water modeling, atmospheric modeling involving surface water estimates, integrated groundwater-surface water (GW-SW) models, and select related modeling tools. Twenty scientists with expertise in groundwater, surface water, atmospheric modeling and/or data management were interviewed. A workshop with 41 attendees, including experts from Canadian and American agencies, was held in Ann Arbor on April 4-5, 2018 to discuss options for approaches to develop a basin-scale GW-SW model.

Key outcomes

Vision for a model

A basin-scale model has good support at a conceptual level and would be beneficial to improve understanding of GW-SW interactions on a Great Lakes basin scale. To develop a vision for the model further, suggested steps include:

a) Identify and consult with stakeholders to identify needs that could be met with a basin-scale model and to build a broad base of support for developing such a model;
b) Identify questions important to the integrity of the Great Lakes-St. Lawrence River Basin Water Resources Compact, including projected future groundwater withdrawals, nutrient flows in GW/SW and potential low flow conditions, which should be considered during model development;

c) Develop a shared, unified model and/or modeling approach and/or model framework for use by Canada and the United States to increase opportunities to build unified approaches and to avoid conflict;
d) Keep in mind multiple scales, from local to regional to basinwide, so the basin-scale model and/or model framework provides boundary conditions/context for other studies on local and regional scales.

Advocacy for GW-SW modeling by the IJC and its boards would assist in building support and engagement. Other IJC initiatives, such as data harmonization, have successfully garnered support and leveraged talent in both countries.

Modeling approach

No single model should be selected at the outset for use by all agencies and researchers to assess water balance on a basin scale. Modeling a complex system such as GW-SW interactions on a basin scale requires a step-wise approach, starting with simplified constructs before moving to more detailed representations. Deconstruction of the problem and a vision for the model are key to any successful modeling initiative. An initiative to develop basin-scale GW-SW models should include:

- Develop a shared conceptual model of the Great Lakes basin hydrologic system;
- Develop data sharing plans and agreements and initiate data harmonization activities, in consultation with stakeholders;
- Develop a basin-scale framework to facilitate interagency collaboration, stakeholder engagement, data sharing and harmonization, inter-comparison studies and, eventually, to play a role in facilitating stakeholder access to data, model code(s), and other information for regional and local-scale studies;
- Prepare to undertake model inter-comparison studies, including protocols, agreed forcing datasets and metrics for results assessment;
- Encourage opportunistic pilot studies using off-the-shelf products to demonstrate the potential to scale-up and/or to collaborate across borders/disciplines/agencies. Also plan for formal pilot studies with sufficient funding to demonstrate the applicability of one or more model codes;
- Basinwide numerical modeling should begin by determining appropriate vertical and longitudinal scales. Applications of complex and simplified models are not mutually exclusive; paired modeling approaches can be used, depending on the question. Uncertainties arise with simple and complex models, so structural and other sources of uncertainty must be characterized to the extent possible.

Data needs and gaps

The discussion regarding data needs was wide-ranging, reflecting various interpretations of the model vision, key questions and potential future applications. Modeling would be feasible with available data if the question(s) were well defined and the uncertainties associated with data gaps and scientific limitations are part of any modeling study. A strategy on data collection is needed, including where and how often to gather data, and reflecting the needs of the question (e.g., operational functions requiring real time data versus scientific research questions). Some specific data gaps were identified as well as current research projects working to resolve specific data gaps.

Future applications

The themes for future applications of a basin-scale model broadly pertained to supporting management, resilience and sustainability of the Great Lakes ecosystem and resource use. Some specific modeling applications identified include:

a) Groundwater contribution to lake-level fluctuations and water balance;
b) Nutrient loading and pathways;
c) Climate change effects on water temperature and environmental flows;
d) Water availability, suitability and sustainability for agricultural use, drinking water, industrial use and ecosystem function;
e) Floodplain function and management.

Challenges and outstanding issues

Several outstanding issues pertain to an initiative to model GW-SW on a basin scale, including:

a) Is the model (are the models) operational or science-based (i.e. intended for research)? What agency/agencies will run it/them? Is there a role for nongovernment organizations?
b) Models need budgets and other resources to stay ‘alive;’ identifying agencies that are mandated to answer the questions posed will be important for sustained support for modeling on a basin scale;
c) Political challenges to having eight states and two provinces agree on a common reporting and data systems. IJC may play a role in facilitating this coordination;
d) The US Department of Energy is working on a comprehensive model that includes the water cycle but limited information was available prior to the workshop for this report.

Recommendations

Management collaboration

A management framework for the initiative should be developed with the flexibility to include and build on research already underway by government agencies and universities, while also tending to the long-term vision of the Science Advisory Board for a modeling platform.

To develop the framework, the form of the initiative should be more clearly defined. For instance, the purpose of the framework may be to establish an environment for model development by a range of actors, including protocols for model comparison similar to the International Panel on Climate Change (IPCC) approach to global climate model development. Alternatively, the framework may be structured to establish a forum for binational collaboration to develop a model or group of models to respond to a set of well-defined questions.

Scientific/technical collaboration

A conceptual model for the surface-subsurface system is needed to facilitate modeling initiatives and inter-model comparisons. The surface watershed perimeter of the basin does not spatially represent the aquifers contributing to the surface water features of the basin (i.e. the lakes, rivers and wetlands); this spatial complexity needs to be represented in a conceptual model for the surface-subsurface system. In addition, a clear need emerged for harmonized, transboundary subsurface information for the Great Lakes basin.

A strategy for data harmonization, data sharing and data access among stakeholders is needed, although the details will depend on the management framework and form of the initiative. Once the model needs are defined inter-modal comparisons should be planned, including common elements to enable direct comparisons.

The core agencies (USGS, NOAA, NRCan, ECCC, MECP, state governments) should encourage opportunistic pilot studies using existing products while strengthening working relationships among researchers.

Preliminary plan

This preliminary plan assumes the preferred approach is to develop a modeling framework that facilitates interagency collaboration, stakeholder engagement, data sharing and harmonization, inter-comparison studies and, eventually, plays a role in facilitating stakeholder access to data, model code(s), and other information for regional and local-scale studies. Although specific GW-SW modeling activities can proceed in an *ad hoc* manner, a framework will better fulfill the Science Advisory Board's vision for a comprehensive modeling platform. The preliminary plan includes support, funding, expertise and core scientific activities.

Support

Endorsement from the IJC through the Science Advisory Board and from the Annex 8 Subcommittee of the Great Lakes Water Quality Agreement is needed to develop a management framework for an integrated GW-SW modeling initiative, including preparation of recommendations for outcomes, budget and schedule, and securing seed funding. With the endorsements in place, an inter-agency steering committee can be established to raise the profile of the integrated GW-SW modeling initiative by consulting with potential stakeholders, funding agencies and others who can contribute in-kind resources. Stakeholders can be engaged to build further support, identify potential funding sources, further define modeling needs, and to refine planned activities to advance the initiative.

Management framework steering committee

An inter-agency steering committee should be assembled to develop the management framework for GW-SW modeling and to report to the IJC through its Science Advisory Board and to the Annex 8 Subcommittee on planned outcomes, resource requirements and schedule. In parallel with the management framework development, the core agencies should support opportunistic studies that are consistent with the objectives to model basin-scale integrated GW-SW interactions and that build inter-agency relationships and capacity.

Conceptual model

In parallel with refinement of the management framework, the agencies responsible for managing groundwater and surface water in the Great Lakes basin should establish a budget with pooled funding to undertake the development of a transboundary hydrologic conceptual model, including stakeholder engagement and refinement of key questions for basin-scale integrated GW-SW modeling. An inter-agency task force of science experts should guide this work.

1 Purpose

This report summarizes the results of a literature review, a survey of science experts and workshop discussions, and suggests an initial action plan to develop an integrated groundwater-surface water (GW-SW) model for the Great Lakes basin.

1.1 Background

In 2000, an IJC report (International Joint Commission, 2000) recommended that governments should take steps to better understand the role of groundwater in the Great Lakes basin. This included research related to data and mapping, consumptive use, the role of groundwater in supporting ecological systems, effects of land use changes and population growth on quantity and quality, groundwater discharge, and estimation of natural recharge areas. The report characterized the interactions between groundwater and surface water to be "frequent and pervasive" and, considering "the virtual impossibility of distinguishing between them in some instances" (p.50), recommended governments apply the precautionary principle in the basin with respect to removals and consumptive use of groundwater (International Joint Commission 2000).

1.2 Project objectives

The Great Lakes Science Advisory Board has identified a need for a basin-scale assessment of the influence of groundwater on water quantity and quality of the Great Lakes basin. This requirement reflects the steadily growing recognition of the significant role of groundwater within the Great Lakes basin (Great Lakes Science Advisory Board to the International Joint Commission 2010). A first step in developing a basin-scale understanding is to develop a satisfactory model of the hydrologic contributions of groundwater to the water balance of the system. While there is some understanding of the contribution of groundwater to quantity and quality at regional scales, there is a gap at the basin scale. Until recently, modeling of surface water and groundwater components has been undertaken for each of these components independently. An integrated water model of surface and subsurface hydrological processes can further serve as the foundation for better understanding of water quality and ecosystem health processes and systems (Grannemann and Van Stempvoort, 2016).

The specific objectives of this project were to:

1. Synthesize knowledge about integrating surface and groundwater models in the Great Lakes region, based on information collected through literature review, a survey of science experts and a workshop of science experts;
2. Identify and document integrated modeling approaches for combined surface and subsurface hydrological processes;
3. Provide recommendations on how to develop an integrated basin-scale GW-SW model.

1.3 Study team

A multi-agency steering committee was assembled by the IJC to guide the project. Co-chaired by the USGS and NRCan, agencies represented included the USGS, NOAA, NRCan, the Ontario government, and three universities. The consulting study team was led by Dr. Mary Trudeau, Director Envirings Inc. with a team that included facilitation services by René Drolet of René Drolet Consulting Services, and subject experts Jim Nicholas of Nicholas-h2o and Dr. Pedro

Restrepo. The consulting team commenced work in October 2017 and the project concluded in June 2018.

1.4 Organization of this document

In addition to this introductory section,

- Section 2 provides a brief overview of the objectives and scope for a basin-scale GW-SW model;
- Section 3 provides a summary of the consulting team's methodology to develop a path forward for an integrated GW-SW model at the basin scale;
- Section 4 summarizes the literature review and survey of science experts;
- Section 5 provides four potential approaches to developing a basin-scale GW-SW model for the Great Lakes;
- Section 6 summarizes the approach to conducting the expert workshop and discussion results;
- Section 7 provides a preliminary plan to develop an integrated GW-SW model;
- Appendices include participants in the expert survey and workshop as well as workshop materials.

2 Model objectives and scope

The first objective for the model contemplated during this project was to better understand the water balance of the Great Lakes on a basin scale. Modeling the interactions of groundwater and surface waters is required to estimate changes in net groundwater storage, along with other components of the water balance, with more reliability than has been implemented to date. Future potential applications for a water balance model were also considered as part of this project.

Knowledge of groundwater's contribution to the water budget for the Great Lakes basin is needed since both direct groundwater discharge (from rocks and glacial sediment to the lakebeds) and indirect discharge (to rivers and streams as base flow) affect water quality and quantity. For instance, contaminated groundwater from various land use activities can have a detrimental effect on potable water supplies, Great Lakes ecosystems, and other water uses. Knowledge of groundwater flow regimes is critical from a water security perspective so sensitive aquifers can be protected from contamination. Understanding the water balance is also essential for better modeling of drought and flood conditions, and for better predicting basin-scale hydrologic changes from changing climatic trends.

The longer-term strategic vision of the Science Advisory Board is to develop an integrated modeling platform that will provide scientific information for the IJC to support the governments of Canada and the United States in maintaining water security and in making decisions on ecosystem management. There are a wide range of modeling approaches that may bridge an integrated GW-SW water balance model and the broader vision of the Science Advisory Board. A vision for the model was discussed with the steering committee in advance of the workshop and also by workshop participants, as documented in Section 6. Discussions naturally highlighted the need for a broader platform that includes stakeholder engagement, data sharing agreements, data and nomenclature harmonization, and collaboration to understand modeling results (such as a shared conceptual model and inter-model comparison protocols).

These very preliminary insights allow a plan to be sketched for the development of an integrated model that will dovetail over the longer term with the integrated modeling platform envisioned by the Science Advisory Board. Identification and selection of the next steps depends largely on the engagement of stakeholders, including the research community, in further defining modeling needs and developing feasible strategies for model development.

3 Methodology

Once initiated, the first phase of work for the project was to undertake a literature review and expert survey. The literature review included government reports and peer-reviewed literature published in academic journals. The scope of the literature review included GW-SW modeling within the Great Lakes basin, and work outside the basin that addressed relevant topics such as modeling glaciated aquifers and modeling techniques. In consultation with the steering committee, 23 science experts were identified from a cross-section of relevant agencies. The interviewees had expertise in groundwater, surface water and/or atmospheric modeling, as well as data management.

Prior to contacting the experts, the consulting team developed a survey instrument and customized it to include summaries of each expert's recent publications. A copy of the customized survey instrument was emailed to each expert in advance of an interview by telephone or Skype. Twenty of the experts (see Appendix A) agreed to participate in interviews that took approximately one hour each. Subsequent to the expert survey, additional literature sources were retrieved for review. Following the workshop, several experts provided comments and clarifications on the literature review.

The second phase of work included planning and delivery of an expert workshop. Workshop invitees were identified by the steering committee, the consulting team, and other experts as the work progressed. A whitepaper was distributed to participants in advance of the workshop with the literature review, options for potential approaches to developing a basin-scale GW-SW model, and key questions for discussion. The potential approaches are summarized in Section 5 and the workshop approach and discussion results are summarized in Section 6. The final phase of work included development of an initial action plan in consultation with the steering committee. This plan is documented in Section 7.

4 Literature review

4.1 Introduction

Since a 2000 IJC report recommending groundwater be studied (International Joint Commission 2000), numerous modeling studies of groundwater-surface water interactions within the Great Lakes basin have been undertaken. However, the geographic focus has been uneven within the basin, with some areas (e.g. Lake Michigan and southern Ontario) receiving more attention than others (e.g. north of Lake Superior). Studies undertaken on a wide range of temporal and spatial scales have had varying perspectives from groundwater to weather prediction. In 2016, an assessment of key scientific questions was prepared for the Great Lakes Water Quality Agreement Annex 8 Subcommittee to the Great Lakes Executive Committee on the topic of GW-SW interactions (Grannemann and Van Stempvoort, 2016).

In reviewing literature on GW-SW interactions, issues of scale and uncertainty regularly arose. An overview of the approaches to GW-SW modeling follows as well as a more detailed review of the literature, organized by type of modeling approach. Methods to support model development or to assist in verification are then outlined, followed by a discussion of key data gaps in the final subsection of this literature review.

4.2 Scale

The influence of spatial scale (point, reach, catchment, aquifer/watershed, basin) and temporal scaling relationships between surface and groundwater processes are not fully understood (Kornelsen and Coulibaly, 2014) in terms of quantity, quality and ecosystem processes. The temporal scale for typical surface water flow modeling (measured in volume per second, minute, hour or day) can differ by orders of magnitude from the temporal scale of groundwater movement (measured in periods of days to centuries). The dominant processes for GW-SW interaction at a local spatial scale may differ from those at a regional scale, but these differences have not been clearly quantified; similarly dominant processes may occur over shorter temporal scales for local issues in comparison with those at larger spatial scales (Barthel and Banzhaf, 2016). For instance, at regional spatial scales, water abstractions could be important to modeling results (Frey, Berg, and Sudicky, 2016) whereas, at a basin scale, the effects are not detectable or are unknown for the period being modelled.

Knowledge of regional scale GW-SW processes is scattered and distributed over a range of different research fields (Barthel and Banzhaf, 2016). Inevitable data issues or limitations contribute further to modeling uncertainty and limitations. According to Barthel and Banzhaf (2016), “knowledge of how to examine GW-SW interactions at the regional scale is mainly derived from studies carried out at local scales, without a clear theory of how upscaling should be performed. There is hardly any evidence that this approach is appropriate” (Barthel and Banzhaf, 2016). However, this statement is contradicted by recent integrated hydrologic modeling review papers that indicate an understanding of many regional processes while also outlining areas for future research (e.g. Fatichi et al. 2016; Clark et al. 2017).

It is also the experience of the USGS in developing the GSFLOW and MODFLOW models that scientists have been able to access numerous hydrologic studies and theoretical approaches for upscaling specific hydrologic phenomena (R. Niswonger, pers. comm. 2018). For example, research on upscaling unsaturated flow at the regional scale indicated that unsaturated flow beneath the soil zone is vertical (Harter and Hopmans, 2004; Z. Chen, Govindaraju and Kavvas, 1994) and this information led to the development of the USGS Unsaturated-Zone Flow (UZF) Package (Niswonger, Prudic and Regan, 2006). Through its research and modeling expertise, the USGS has implemented other regional scale modeling approaches, including simulation of the water table at the regional scale using the sub-grid scale (with saturated thickness referenced using the water table, not the cell thickness) and stream geometry being defined at the subgrid scale rather than using the model cell area (R.Niswonger, pers. comm.2018).

Atmospheric conditions are influenced on a global scale, hydrology on a regional scale, and groundwater on a local to regional scale. Global Water Futures (GWF) and many other researchers are working to identify appropriate scaling interrelationships for modeling purposes (A. Pietroniro, pers. comm. 2017).

Scale terminology is not always consistent from one study to the next, but guidelines to spatial scale terminology within the academic literature on GW-SW interactions (after Barthel and Banzhaf, 2016) include:

- Point scale is the smallest spatial entity, such as the influence of one well.
- Local scale refers to the interaction between one surface water reach and the adjacent alluvial aquifer.
- The terms sub-catchment, small catchment and watershed have no defined scale but the study areas encompass a drainage area smaller than the regional scale.
- The term regional scale as used in academic literature refers to catchments larger than 100 km^2.

In this literature review, regional scale refers to part or all of a Great Lake catchment or aquifer, whereas basin scale refers to all five lakes and their catchment areas and associated aquifers. Temporal scale issues are not explored in depth within the literature review.

4.3 Uncertainty and limitations for modeling groundwater

The spatial and temporal variability of groundwater and surface water flows necessitates simplifying assumptions in all models. Uncertainties and limitations are inherent in GW-SW modeling in terms of the science, modeling methods and data gaps, quality and availability. Uncertainty must be addressed using an appropriate framework, and the framework requires a systematic approach to rank sources of uncertainty in terms of their effect on the outcomes of interest (Fatichi et al. 2016).

To understand the water balance of the Great Lakes basin, calculations for each component of the balance must include estimated uncertainties, while also recognizing the inherent uncertainty of such estimates. In desktop calculations of the net groundwater component of the Great Lakes water balance, without adequate estimation of uncertainties associated with each component, the accumulated error ends up in the calculated net groundwater changes, bringing into question the validity of calculated net groundwater changes (Wiebe et al. 2015) using methods that do not include groundwater models.

Groundwater modeling is needed to understand the groundwater components of the Great Lakes water budget. Further, researchers have called for a more systematic and consistent approach to model verification and skill assessment (Gronewold and Fortin, 2012). Quantitative frameworks and metrics, such as those provided by parameter estimation, are central to model development, calibration and sensitivity assessment. For complex models, advanced statistical metrics are needed to understand how the model represents variation in the underlying assumptions. One tool to assist in parameter estimation is PEST (Doherty 2002), as described further in Section 4.11.

4.4 Overview of approaches and methodologies to modeling GW-SW interactions

Groundwater-surface water interactions are included in atmospheric and weather prediction models, in surface hydrology models, in groundwater models, and in more complex groundwater-surface water models. The treatment of groundwater flows within a model depends on the model objectives. For instance, weather prediction models simplify groundwater flows because groundwater does not have short-term influences on atmospheric forcings. On the other hand, groundwater flow modeling is the prime objective of studies concerning groundwater resources, such as risk assessment for groundwater extractions.

Table 4.1 provides a summary of the modelled variables influencing the interaction of groundwater with surface water, organized by system 'layer' (atmosphere, surface, vadose, ground). Figure 4.1 (overleaf) provides a simplified conceptual visual summary of the typical range of models in the literature review that include aspects of GW-SW interactions.

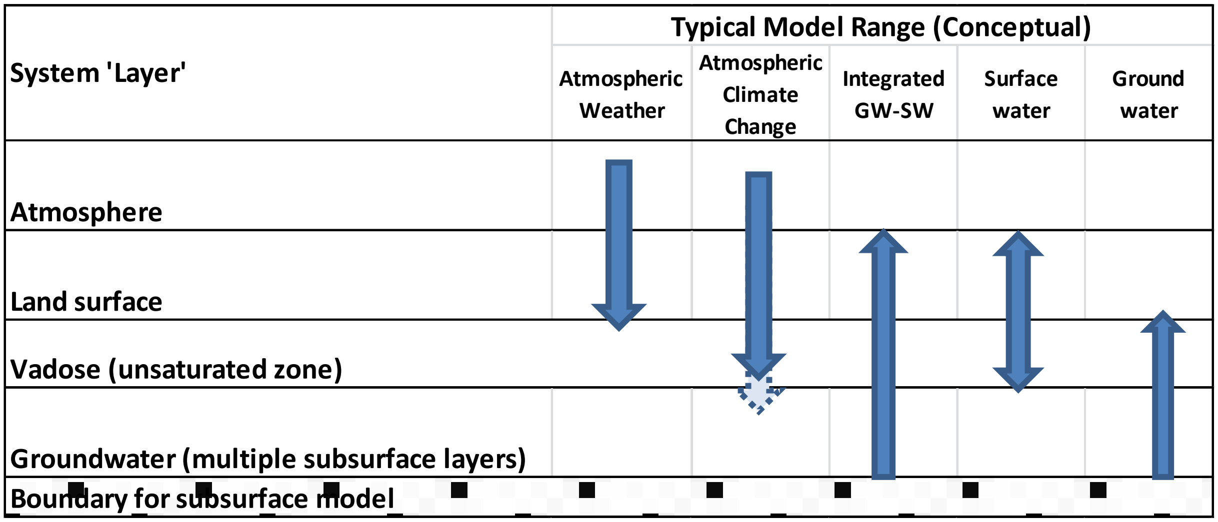
Table 4.1 Overview of modelled variables influencing the interaction of groundwater with surface water

System 'layer'	Variables influencing lower layers	Variables influencing upper layers	Conditions that add complexity
Atmosphere	Variables affecting evapotranspiration (e.g. wind speed; air temperature; radiation); precipitation	Not applicable	Climate change
Land surface	Vegetation/transpiration; hydraulic head/surface water elevations; storage (e.g. lakes); land cover/use; surface characteristics (e.g. slope, roughness)	Vegetation/transpiration; Land cover roughness and thermal properties	Wetlands; water taking; ice/snow cover and melt; large lakes (ice conditions, evaporation); snow/blowing snow
Vadose (unsaturated zone) This layer may not be present in some locales	Soil moisture retention; capillary barrier effects; roughness	Soil moisture retention; capillary barrier effects; roughness	Drought conditions; water taking; drainage; ice/snow cover and melt; natural soil/surface variability and characteristics
Groundwater (multiple subsurface layers)	Not applicable	Hydraulic conductivity; hydraulic head; storage properties (e.g. specific yield); bedrock permeability; vertical dispersivity and molecular diffusion (for solute transport)	Karst formations; exposed rock (e.g. Canadian shield); depth of denser water layers (saline conditions); water taking; aquifer heterogeneity (e.g. glacial till)
Boundary for subsurface model	Not applicable	Assumed to be none/insignificant for model purpose	Scale(s) of analyses

The level of modeling detail required for each system ‘layer’ depends on the model objectives, which, in turn, determine the degree to which linkages between upper and lower system layers are included. For instance, atmospheric weather forecasting models incorporate wind speed and direction, humidity, pressure, short and long wave radiation, land surface roughness, and other variables to predict atmospheric energy fluxes, precipitation and temperature. These models do not rely on detailed groundwater information, day-to-day land use conditions, or hydraulic head to make weather forecasts, although they may use soil parameters.

On the other hand, atmospheric models with an objective to predict climate change effects may require several soil, hydraulic head and groundwater variables to predict low flow or drought conditions. Integrated GW-SW models require atmospheric inputs, such as precipitation and evapotranspiration to simulate changes in vadose saturation and surface water levels, but they typically do not attempt to feed atmospheric models in terms of energy fluxes, nor do they require wind speed and other atmospheric forcings in their configurations.

Figure 4.1 Simplified conceptual visual summary of the typical range of models in the literature review



Groundwater and surface water models can be integrated but the terminology for model coupling is not precisely defined. AquaResource identifies three configurations for integrated models: externally-coupled (surface water and subsurface equations are solved separately and in succession without iteration within a time step); iteratively-coupled (surface water and subsurface equations are solved separately but iteratively within a time step, proceeding to the next time step when the iteration errors drop below a prescribed threshold); and fully-coupled (surface, subsurface and fluid fluxes are solved simultaneously at each time step) (AquaResource Inc. 2011).

The National Groundwater Association (NGWA) identifies three model coupling options: manually-linked modeling; coupled modeling; and, fully-integrated modeling (NGWA 2017). Paniconi and Putti (2015) use the term loosely-coupled to mean one-way passing of information among sub-models and tightly-coupled to mean coupled equations and feedbacks. Maxwell et al. (2014) use three terms for surface-subsurface hydrologic models: sequentially iterative (a time-splitting approach where lagged variables are used in iteration until convergence); global implicit (all variables are used in a single nonlinear system of equations); and asynchronous linking (progresses in time by lagging the dependent variables so various governing equations can be solved asynchronously) (Maxwell et al. 2014). Barthel and Banzhaf (2016) use two simple terms to identify configurations for model coupling: loosely-coupled models and fully-coupled models. Manual coupling is an option that may be used in the preliminary development stages for complex models (AquaResource Inc. 2011), for example to scope data needs or to understand potential parameter ranges.

These variations in terminology can cause the same models to be categorized differently. For example, Barthel and Banzhaf (2016) identify MIKE SHE and CATHY as two examples of loosely-coupled models (distinct from fully-coupled models HGS and ParFlow), yet NGWA identifies these two models as fully-integrated and comparable to HGS and ParFlow (NGWA 2017). AquaResource identifies HydroGeoSphere (HGS), ParFlow (and a third model, MODHMS) to be fully-coupled but GSFLOW and MIKE SHE to be externally-coupled (AquaResource Inc. 2011).

For our purposes the following definitions are used, which are most closely aligned with the AquaResource definition:

> **Fully coupled**: models that integrate surface and groundwater processes by simultaneously solving equations representing the various physical processes. This approach avoids the need for interfaces between separate model modules (Barthel and Banzhaf, 2016). These models fall within the fully-coupled definitions by AquaResource and Barthel and Banzhaf; they are a subset of fully-integrated models within the NGWA definition.This model type is called *globally implicit coupling* by Maxwell et al. (2014).
>
> **Externally and iteratively coupled**[1]: models that solve for surface and subsurface processes separately– either in succession without iteration within a time step (including models that are one-way linked with no feedback) or iteratively within each time step (AquaResource Inc 2011). These models are both the externally-coupled and iteratively-coupled models in the AquaResource definition and loosely-coupled models in the Barthel and Banzhaf definition. In the NGWA definition, all coupled models and some fully-integrated models fall into this category. Loosely-coupled model options vary widely, depending on the models and methodologies selected.

It is outside the scope of this project to recommend any particular model code but it is useful to appreciate the variability among models when developing an action plan for next steps. In addition to coupling configurations, models also vary in their treatment of exchanges at boundaries between groundwater, the vadose zone and the atmosphere. Fundamentally, models may use structured (e.g., finite difference) or unstructured (e.g., finite element) grids. Various models take differing approaches to representations of terrain and in their flexibility to alter spatial scales (e.g., fixed grid size versus the option for denser grids in complex landscapes, such as along rivers.) For instance, GSFLOW represents stream channels geometries at the subgrid scale (in cm), within a much larger model cell (hundreds of meters) so that, at regional scales, stream depth can be simulated as well as SW-GW exchanges (R.Niswonger pers. comm. 2018). Similarly, the range of available time step increments varies. Some models have the capability to simulate snow, ice and snow melt conditions. Some models extend the surface/subsurface coupling to solute transport (e.g., HydroGeoSphere and CATHY), erosion and sediment transport (tRIBS), and thermo-mechanical processes (OpenGeoSys) (Paniconi and Putti, 2015).

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[1] Note that in the workshop discussion white paper, the term ‘loosely-coupled’ was used for this group of models; several groundwater experts indicated the Barthel and Banzhaf (2016) use of the term ‘loosely-coupled’ was vague and potentially confusing or misleading.

Intercomparison studies have examined the trade-offs of various coupling options and the performance of models under theoretical or small-scale case studies (Fiorentini, Orlandini and Paniconi, 2015; Maxwell et al. 2014; Kollet et al. 2017; AquaResource Inc. 2011).

For the literature review, models to simulate GW-SW interactions are grouped into five categories based on their central focus and coupling type:

1. *Surface water models*. These models take a simplified approach to the atmospheric and groundwater components but they can be coupled (externally, iteratively or manually) to models of other components. Examples are numerous, including the USGS's PRMS model and NOAA's National Weather Service models in the Community Hydrologic Prediction System.

2. *Groundwater models*. These models, with the exception of base flow estimation, take a simplified approach to the atmospheric and storm-related surface water components, but they can be coupled (externally, iteratively or manually) to other models of those components. An example is the USGS's MODFLOW.

3. *Manually linked models*. This modeling approach includes models in the two previous groups. Manually linked approaches may be used to assess simplifying assumptions in advance of building more complex models (AquaResource Inc. 2011). They may also suffice for modeling purposes that are not driven by short-term transience (R.J. Hunt and Steuer, 2001).

4. *Externally and iteratively coupled models*. This group of models is the largest of the five categories because it includes a variety of approaches to combining the results of two or more models. The approach includes atmospheric models that use land surface models to simulate hydrologic contributions to atmospheric conditions from surface waters/groundwater; in these cases, GW-SW interaction elements include evapotranspiration and soil conditions. The approach also includes models that begin with groundwater or surface water simulations and build connections from that base. An example of a model in this group is the USGS' GSFLOW, which links PRMS and MODFLOW.

5. *Fully coupled groundwater-surface water models (also called fully integrated models)*. These models simultaneously solve process-based equations for groundwater and surface water systems within one model code. Examples include: ParFlow, HGS, InHM, and OpenGeoSys (Barthel and Banzhaf 2016); MODHMS (AquaResource Inc 2011); and, CATHY and tRIBS (Maxwell et al. 2014).

4.5 Overview of the scale addressed in studies relevant to the Great Lakes basin

The spatial scale of models relevant for the Great Lakes basin range from very small (e.g., 10 km^2) to continental (e.g., Canada-wide, see Chen 2015). Within this range, the smaller scale (i.e., subwatershed or reach scale) clearly dominates in terms of frequency of model development. In particular, numerous surface water models have been developed at smaller scales for hydrology, water quality, pollution transport, and erosion assessments for US Great Lakes tributaries (Coon et al. 2011) and Ontario municipal water supply subwatersheds. There is no central inventory of Ontario surface water or groundwater models; a study by Coon et al. (2011) inventoried models for tributaries to the US Great Lakes. Models for tributaries to Lakes Michigan and Erie accounted for over 65 percent of the models for all lakes and connecting channels in the Coon et al (2011) inventory.

Two models, the US National Water Model and Canada's Water Cycle Prediction System, can provide inflow forecasts for basin lakes on both sides of the border, but neither incorporates sophisticated hydrological models. Atmospheric models use Land Surface Models (LSMs) that simulate surface hydrology at a fairly coarse resolution with simplifying assumptions for groundwater and soils. Only the Lake Michigan basin has a regional scale (i.e., an entire lake basin) groundwater model, which was developed by the USGS (Reeves 2010). The USGS also developed a surface water model using the same model domain as the Lake Michigan MODFLOW model (Reeves 2010). A proof-of-concept fully coupled model (using HGS) is in the early development phase for southern Ontario (Frey, Berg, and Sudicky 2016). Other fully coupled models have been developed at much smaller scales, i.e. for short reaches or small subwatersheds in the range of one to two hundred square kilometers, and for the Grand River (Ontario) which is ~7,000 km^2.

4.6 Surface water models

In 2005, the USGS, in cooperation with Environment Canada[2], released *Base flow in the Great Lakes Basin* (B P Neff et al. 2005), a study of daily streamflow records from gauging stations in Ontario and the eight Great Lakes states. *Estimation of shallow ground-water recharge in the Great Lakes Basin* (2006) (B P Neff, Piggott, and Sheets 2006) developed an approach to estimate long-term average recharge rates; however, the approach is not able to estimate the variability of recharge over relatively short time scales (B P Neff, Piggott and Sheets, 2006). In 2014, the USGS simulated basin-scale climatic and hydrologic conditions in the Lake Michigan basin for current and forecast scenarios using the Precipitation-Runoff Modeling System (PRMS) model (Christiansen, Walker and Hunt, 2014). Groundwater is conceptually simplified in PRMS as a group of parameters that control runoff, infiltration into the soil zone, and the rate and volume of flow from groundwater to surface water (Christiansen, Walker and Hunt, 2014). PRMS (Markstrom et al. 2015) and GSFLOW, discussed in Section 4.9, simulates lateral flows, including lateral overland flow and lateral subsurface flows in the soil zone that can cascade among cells on the landscape or to a stream, lake, or wetland; unsaturated flow beneath the soil zone is vertical over cells at the scale of tens of meters (Harter and Hopmans, 2004; Z. Chen, Govindaraju and Kavvas, 1994), a property that is simulated in regional and basin scale PRMS and GSFLOW models (R.Niswonger, pers. comm. 2018 and see Cascade Routing Procedure in Markstrom et al. 2015).

For US Great Lakes tributaries, numerous surface water models developed by NOAA, the US Army Corp of Engineers, academics, and others assess hydraulic, sediment, or water quality conditions on a subwatershed or reach scale (Coon et al. 2011). Models used include: the Soil and water assessment tool (SWAT); Hydrologic engineering center river analysis system (HEC-RAS); Long-term hydrologic impact assessment (L-THIA); Pollutant Loading (PLOAD); Annualized agricultural nonpoint source pollution model (AGNIPS); Analysis of flows in network channels (AFINCH); Water availability tool for environmental resources (WATER); Water erosion prediction project (WEPP); High impact targeting (HIT); Integrated landscape hydrology model (ILHM); and Hydrological simulation program - Fortran (HSPF) (Coon et al. 2011). In an inventory for the US Great Lakes by Coon et al (2011), over 90 percent of the

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[2] Environment Canada's name has changed to Environment and Climate Change Canada (ECCC). In this report, the names of government departments cited are the names at the time the reports were written for ease of retrieving references.

inventory are models of surface water flows or related processes (e.g., sediment transport, pollutant transport).

The USGS study, *Water availability and use pilot: A multiscale assessment in the U.S. Great Lakes basin* (2010), included surface water flow modeling using a spatial regression approach. The surface water application AFINCH was applied to a subregion of the Lake Michigan basin to estimate monthly streamflow and water yields, including within ungauged areas (Reeves 2010; Feinstein, Hunt and Reeves, 2010). AFINCH is a simple regression model based on measured surface water flows (R. Hunt, pers. comm. 2018).

The USGS study, *Estimation of monthly water yields and flows for 1951-2012 for the United States portion of the Great Lakes basin with AFINCH* (2014), estimated monthly water yields from 105,829 catchments and corresponding flows in 107,691 stream segments. The US portion of the Great Lakes basin was partitioned into seven hydrologic subregions and the monthly water yields and flows in each study area were estimated (Luukkonen et al. 2015).

Numerous local-scale surface water models were developed by Conservation Authorities and municipalities in Ontario to comply with required risk assessment for municipal water supplies, per the provincial *Clean Water Act* (2006). For instance, a HSPF was used in the Orangeville area of southern Ontario for this purpose (AquaResource 2013). Model codes, datasets and results are housed by the respective Conservation Authorities and/or municipalities responsible for each Surface Water Protection Area and potable water supply system.

A high-level model for all Canadian watersheds of Lake Erie has just been completed (pending publication[3]) using SWAT to determine water balance (P. Goel, pers. comm. 2017). SWAT is a watershed scale model that uses a daily time step to simulate hydrology, sediment and water quality (Golmohammadi, Rudra, Dickinson, et al. 2017). SWAT has also been applied to local scale watersheds (e.g., the Gully Creek watershed (10.5 km^2) (Golmohammadi, Rudra, Dickinson, et al. 2017) and to model local-scale agricultural lands by incorporating DRAINMODE into SWAT to compute the soil water balance (Golmohammadi, Rudra, Prasher, et al. 2017). Surface water models such as SWAT focus on a couple of meters of the top soil layer (P. Goel, pers. comm. 2017). Winter and spring hydrology are not well represented in surface water models (i.e., the smaller scale processes are generally not well represented) (P. Goel, pers. comm. 2017).

4.7 Groundwater models

The Michigan Basin Regional Aquifer System Analysis (RASA) project (circa 2000) developed a MODFLOW (steady-state-finite-difference) model of the groundwater system that is defined by the extent of bedrock units in Michigan's Lower Peninsula, bounded by a continuous specific-head boundary formed from Lakes Michigan, Huron, St. Clair, and Erie, with the St. Clair and Detroit River connecting channels (Hoaglund, Huffman, and Grannemann 2002). The model estimated groundwater recharge to a simulated water table, and estimated direct (riparian) and indirect (stream base flow) groundwater discharges to three Great Lakes from the Michigan Lower Peninsula (Hoaglund, Huffman, and Grannemann 2002). The estimated direct groundwater discharges to the lakes in this study were higher than a 2010 USGS study due to the

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[3] The paper was published in February, 2018: Daggupati et al., 2018. Hydrological Responses to Various Land Use, Soil and Weather Inputs in Northern Lake Erie Basin in Canada, *Water*, 10 (222).

boundary conditions used (N.Grannemann, pers. comm., 2018). Also as part of the RASA project, a model for the regional groundwater flow and geochemistry was developed for the Midwestern Basins and Arches aquifer system in parts of Indiana, Ohio, Michigan, and Illinois (Eberts and George 2000).

A 2010 USGS Great Lakes Pilot Study publication (Reeves 2010) summarized the results for a regional groundwater flow model for the Lake Michigan basin and a local-scale analysis of groundwater-surface water interaction for a small (~21 mi^2) inset within the Lake Michigan basin. The subregional groundwater flow model quantified groundwater availability and simulated responses to stresses for the Lake Michigan basin using MODFLOW-2000 for groundwater flows and SEAWAT-2000 to represent the effect of salinity and density-dependent flow within the cone of depression that extends into saline parts of the Michigan basin (due to groundwater pumping adjacent to the Great Lakes basin) (Reeves 2010).

The Soil-Water-Balance (SWB) model was used to estimate water delivered through the soil zone to the water table (Reeves 2010; Westenbroek et al. 2010). Increasing the number of surface water features in the model constrains (as boundary conditions) the water table solution developed by the model, thus setting up a trade-off between representation of surface features and usefulness of the model to simulate conditions that alter the shallow groundwater system (such as pumping) (Feinstein, Hunt and Reeves, 2010). Recognizing issues with regional discretization scales, the Lake Michigan basin regional model was used as the basis to estimate water available to wells and springs for the Kettle Moraine Springs State Fish Hatchery in Wisconsin (Dunning et al. 2017). In a 2017 study, the USGS applied the SWB to the glaciated regions of the contiguous United States, which includes the entire extent of the US side of the Great Lakes basin (Reeves et al. 2017). Results of this modeling effort were compared to results of two other recharge estimation methods applied across the glacial system (results pending publication, S. Eberts pers. comm., 2018).

The MODFLOW code is updated regularly with versions differentiated by a hyphenated suffix. MODFLOW-NWT (Niswonger, Panday and Ibaraki, 2011) was developed from MODFLOW-2005 for applications to thin model layers under unconfined conditions (Feinstein et al. 2012). MODFLOW-NWT was used for the Fox River, a tributary within the Mississippi River basin (i.e., not within the Great Lakes basin) with the streamflow/lake (SFR/LAK) packages to represent groundwater-surface water interactions (Feinstein et al. 2012). The intent of the two models was to increase understanding of the uncertainty inherent in model results and predictions since neither model is a true representation of the subsurface (Feinstein et al. 2012). MODFLOW-NWT was used in 2016 for the Bad River (~1000 mi^2), a tributary to Lake Superior in Wisconsin, to evaluate groundwater-surface water interactions (Leaf et al. 2015). In that study, MODFLOW-NWT simulated steady-state groundwater flow, while base flow in streams was simulated using the streamflow routing (SFR) package (Leaf et al. 2015). In 2016, a semi-structured MODFLOW-USG model was used to provide statistical measures of the correlation between modeled inputs and simulated surface water depletion in response to shallow well pumping (see also the metamodels subsection below) (Feinstein et al. 2016). In a 2017 USGS study, MODFLOW was used for a modeling study in Wisconsin that had the express purpose of exploring information loss with loss of model complexity (Juckem, Clark and Feinstein, 2017). In that study, three groundwater flow models were developed with differing levels of complexity to assess the effects of model complexity on simulated water levels and base flows in the glacial aquifer system (Juckem, Clark and Feinstein, 2017).

MODFLOW has also been used for applications in Ontario as part of the provincial initiative to characterize drinking water source protection (under Ontario's *Clean Water Act, 2006*). For instance, three towns in the region of Orangeville, Ontario used MODFLOW to assess the water balance as part of risk assessment requirements under that act (AquaResource 2013). Ontario has numerous models developed for source protection (S. MacRitchie, pers. comm. 2017). The data, models, and results are not compiled in a central location. However, in support of the development of a southern Ontario regional modeling platform (see Frey, Berg and Sudicky, 2016), the Geological Survey of Canada is mining data from these numerous reports, including detailed hydrogeologic information and borehole information (S. Bates, pers. comm. 2017). Ontario is also developing plans and other projects under the *Lake Simcoe Protection Act* (S. Bates, pers. comm. 2017).

The Conservation Authorities Moraine Coalition (CAMC), made up of four municipalities and nine conservation authorities north of Lake Ontario, lie within the 160 km long Oak Ridges Moraine, a recognized regional groundwater recharge area (AquaResource 2013). The CAMC has assembled a database, constructed a regional geologic framework representing the geological layers, and developed numerical groundwater flow models to assist in water management decision making (AquaResource 2013). A MODFLOW model simulated movement of groundwater into small tributaries and rivers that could additionally lose water back to the aquifers (AquaResource 2013). This group is also notable for its comprehensive approach to data sharing and collaboration protocols (S.Bates, pers. comm. 2017).

The Chateauguay River watershed (along the Quebec-New York State border), a tributary to the St. Lawrence River with an area of 2,850 km^2 (1,100 square miles), was modelled using FEFLOW (Blanchette et al. 2010). This numerical model was used to simulate stress and climate scenarios for the Chateauguay River watershed (Lavigne, Nastev and Lefebvre, 2010). An ongoing project in southern Quebec, south of the St. Lawrence River, focuses on assessing the impacts of climate change on groundwater resources, but also with an emphasis on the relationship between surface water and groundwater (R. Lefebvre, pers. comm. 2017).

Hydrogeological and geochemical data were gathered to develop a comprehensive transboundary conceptual model of the Milk River aquifer (Alberta-Montana) (25,000 km^2), to build on a previously developed unified geological model, and in preparation for the future development of a numerical 3D groundwater flow model of the aquifer (Pétré et al. 2016). The mathematical model will be used to test the conceptual model and to propose management actions for the groundwater resource (Pétré et al. 2016). Various datasets along the US-Canada border were harmonized and are stored by respective government agencies in Canada and the United States (Pétré et al. 2016). The approach used in this study may be applicable for the Great Lakes basin.

Groundwater modeling using analytic element technique

Analytic element modeling does not require a grid or cells (Juckem, Fienen and Hunt, 2014). An infinite aquifer is assumed; important groundwater flow control features, such as wells and surface water features, are represented as mathematical elements or strings of elements (Juckem, Fienen and Hunt, 2014). This approach was used in 2005 to model Lake Ontario (Craig, Jankovic and Barnes, 2006). GFLOW, a 2D steady-state analytic element groundwater flow model was constructed for the Lac du Flambeau Reservation, Wisconsin to assess various wastewater management approaches and water quality effects (Juckem, Fienen and Hunt, 2014). In 2016, a hybrid MODFLOW-analytic element-groundwater flow model using GFLOW (H. M. Haitjema 1995) was applied to a watershed in the Lake Michigan basin (Abrams et al. 2016).

The analytic element approach was less labour intensive than development of an inset model (Juckem, Clark and Feinstein, 2017). In the Great Lakes region, most of the transmissivity is in the upper layer (R. Hunt, pers. comm. 2017). Because the top layer (the analytic element layer) has the bulk of system transmissivity, the solution can be attained without iterating between GFLOW and MODFLOW so run times are shorter (Haitjema et al. 2010). If transmissivity is in the deep layer, run times would increase (Abrams et al. 2016; Haitjema et al. 2010). When transmissivities in the deeper layers dominate, iterative procedures to couple the GFLOW and MODFLOW models are needed at additional computational cost (Haitjema et al. 2010). A consideration in applying the analytic element method is that it is not well suited for highly heterogeneous aquifers and highly transient settings (Hunt 2006). For instance, the analytic element approach is difficult to apply in systems with strong nonlinearities, including exchanges between SW-GW that significantly affect the depths and storages in surface systems (R. Niswonger, pers. comm. 2018). Modeling objectives need to be assessed in making the decision to adopt analytic elements or to proceed with modeling approaches suited for a wider range of hydrologic settings (R. Hunt, pers. comm. 2018; J. Starn pers. comm, 2017).

4.8 Manually linked models

This approach is used as an initial step in developing more complex models. For instance, see the manually linked step described in Section 4.9 (Groundwater base) documented in the USGS report, *Simulation of climate change effects on streamflow, lake water budgets, and stream temperature using GSFLOW and SNTEMP, Trout Lake Watershed, Wisconsin.* Simulated stream flows from the GSFLOW model and other basin characteristics were used as input to the one-dimensional Stream-Network TEMPerature (SNTEMP) model to simulate daily stream temperatures in selected tributaries (Hunt et al. 2013). GSFLOW can be run so that the PRMS model is separate from the MODFLOW or active in some areas of the model and not in others (R. Niswonger, pers. comm. 2017).

As part of the USGS study, *Water availability and use pilot: A multiscale assessment in the U.S. Great Lakes Basin* (Reeves 2010), a desktop regional water budget analysis for the Great Lakes basin was undertaken using existing information sources (in particular, *Uncertainty in the Great Lakes water balance*, (Neff and Nicholas, 2005) to estimate stocks and flows based on long-term temporal averages (Reeves 2010).

4.9 Externally and iteratively coupled models

These modeling approaches may use a combination of process-based models only, or process-based models and other algorithms or empirical relationships. The output from one or more individual models becomes the input for one or more other models. An advantage of these approaches is the relative simplicity of individual models to enable multiple runs of the component models for calibration and uncertainty analyses. The model structure allows for flexibility in terms of models and sources of inputs to the base model.

A disadvantage of externally coupled models can be disagreements among the individual models when they are calibrated independently. Convergence can be an issue in any nonlinear model, including iteratively-coupled models, but these problems can be compounded by degradation of the flow solution if too large a time step is specified (AquaResource Inc 2011). In addition, long runtimes can artificially force a modeler to limit the model parameters used for calibration and uncertainty analysis (e.g. Doherty and Hunt, 2010). To address this issue, a sequential, iterative approach may be required as an interim calibration step in a coupled model calibration, providing a better starting point for calibration of the slower running fully coupled model, which speeds calibration (e.g., the USGS study for Trout Lake (Hunt et al. 2013) identified below). Another potential disadvantage is that the modeling team must be familiar with more than one code. Similar to the fully coupled models, process-based models typically have numerous estimated parameters and associated uncertainties.

The literature for this broad category is summarized in two groups: groundwater base and surface water/atmosphere base. In their review of regional GW-SW models used around the world, Barthel and Banzhaf (2016) found that (in their terminology) *loosely coupled* models were more commonly based on surface water models than on groundwater models. Typically the base model comprises the most advanced aspect of a regional study, whether a surface (i.e., rainfall runoff) model or a groundwater flow model, and the other part is represented through relatively simple conceptual design (Barthel and Banzhaf, 2016).

Groundwater base

Where a groundwater model formed the basis for externally and iteratively coupled models in a global literature review, the USGS' MODFLOW program was the model code most frequently used for this purpose (Barthel and Banzhaf, 2016). MODFLOW is the groundwater model in the USGS' GSFLOW model. (Note that GSFLOW is based equally on a surface water and groundwater model.) Commercially available (proprietary) DHI products, FEFLOW coupled with MIKE 11, and MIKE SHE, were also commonly used for regional studies globally using coupled model configurations (Barthel and Banzhaf, 2016). The surface water discharge and soil moisture models used to couple with MODFLOW vary in complexity.

The USGS study, *Water availability and use pilot: A multiscale assessment in the U.S. Great Lakes Basin* (2010) included a subregional analysis of consumptive water use. For the local scale assessment of groundwater-surface water interactions, the 5.44 m^2 (21 square miles) inset model was designed in accordance with the requirements for accurate representation of streamflow depletion caused by groundwater pumping (Reeves 2010). The local model required refined geometry and a more detailed modeling package, the Stream-Flow Routing package (SFR1), to simulate stream flow from areas outside the inset model domain; monthly flows from AFINCH were used (Reeves 2010).

The study, *Simulation of climate-change effects on streamflow, lake water budgets, and stream temperature using GSFLOW and SNTEMP, Trout Lake Watershed, Wisconsin* (Hunt et al. 2013), which is located adjacent to the Great Lakes basin, took the approach of precalibrating uncoupled models to construct a better-informed starting point for coupled model calibration; the product was a coupled transient groundwater/surface-water model, GSFLOW, for an area of 310 km^2 (120 square miles) (Hunt et al. 2013).

PRMS used atmospheric forcings, at land surface and within the soil zone, and a groundwater-flow model (MODFLOW-NWT (Markstrom et al. 2008a)) that represented the unsaturated zone, saturated zone, stream, lake budgets and stream temperatures (Hunt et al. 2013). Initially, calibration of the individual models was planned; however, this approach did not provide a sufficiently accurate starting point for efficient coupled model calibration (Hunt et al. 2013). A sequentially linked approach was used to link PRMS-only and MODFLOW-only models for highly parameterized parameter estimation, providing better calibration starting points for the calibration of the less parameterized/slower running coupled model (Hunt et al. 2013).

GSFLOW simulated interaction feedbacks of the surface water and groundwater systems that would not have been achieved with an uncoupled modeling approach; specifically, the model simulated the interplay of atmospheric drivers, Dunnian overland flow, unsaturated zone buffering, and lagged groundwater-system mitigation on lake stage changes (Hunt et al. 2013). A similar approach was used in the 2016 study for Black Earth Creek, Wisconsin (267 km² or 103 square miles), a subwatershed to the Mississippi system (Hunt et al. 2016). The models used and the approach were essentially the same as the Trout Lake Watershed study, except the results from the uncoupled PRMS-only and MODFLOW-only models provided a sufficiently accurate starting point for calibration of the final coupled transient GSFLOW model (Hunt et al. 2016).

Other studies in the United States, outside the Great Lakes basin, have used GSFLOW to simulate the role of surface water-groundwater interactions in snow dominated regions (Huntington and Niswonger, 2012), water budgets and recharge area simulations (Fulton et al. 2015), and shallow groundwater flows in an irrigated alluvial aquifer system (Bailey et al. 2013), among others. GSFLOW can be combined with satellite imagery, geospatial data sets, hydrologic tracers and age dating, and other quantitative and qualitative information for hydrologic prediction (Markstrom et al. 2008b). The USGS Water Availability and Use Science Program (WAUSP) is updating quantitative assessments of groundwater availability in areas of critical importance (including the Lake Michigan basin) and the scale of many of these assessments will be similar to the Great Lakes basin (R. Niswonger, pers. comm. 2017). A map summarizing the critical locations is available at URL: https://water.usgs.gov/ogw/gwrp/activities/regional.html.

Surface water/Atmospheric base

The NEXSS model (*Networks with EXchange and Subsurface Storage*) was developed specifically to simulate hyporheic exchange at a regional scale (Gomez-Velez and Harvey, 2014). The model discretizes a river network into reaches and prescribes geomorphologic characteristics, such as bankful channel width; physically based models are incorporated to simulate vertical and lateral exchange (Gomez-Velez and Harvey, 2014). Simulations indicate that vertical exchange beneath submerged bed forms dominates hyporheic fluxes along river corridors, although lateral exchange through meander banks may be relatively important in large rivers (Gomez-Velez and Harvey, 2014).

The NOAA Advanced Hydrologic Prediction System (AHPS)[4] and Canada's Water Cycle Prediction System (WCPS) are the only two systems that can provide inflow forecasts for each of the Great Lakes on both sides of the Canada–US border; neither relies on very sophisticated hydrological models (Gaborit et al. 2017). Many other forecast models are available, but their spatial domains are typically only within the United States or Canada.

MESH is Environment and Climate Change Canada's (ECCC) Land Surface-Hydrology Modeling System, which has three components: (1) the Canadian Land Surface Scheme that computes the energy and water balance using physically based equations for soil, snow and vegetation canopy; (2) lateral movement of soil and surface water to the drainage system using one of two algorithms (WATROF or PDMROF); and, (3) WATFLOOD for hydrological routing through the drainage system (Yassin et al. 2017). The MESH regional hydrological model was calibrated on the St. Lawrence River basin at Montreal, which includes all of the Laurentian Great Lakes plus the Ottawa River basin; modelled watersheds ranged from 386 km^2 (149 square

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[4] Note that the National Water Model acronym AHPS is the Advanced Hydrologic Prediction Service, which is composed of models, service delivery and other features.

miles) to 16,332 km^2 or 6306 square miles (Pietroniro et al. 2007). MESH has a simplified groundwater model (B. Davison, pers. comm. 2018); however, the Global Water Futures (GWF) project is considering coupling a groundwater model to MESH to assess interactions with groundwater and to identify recharge and discharge areas (A. Pietroniro, pers. comm. 2017). The Great Lakes are one of seven basins across Canada included in the GWF project (A. Pietroniro, pers. comm. 2017). MESH is the surface hydrology application of MEC (Modélisation Environnementale communautaire) (Pietroniro et al. 2007). MEC combines different soil-vegetation atmospheric transfer schemes (SVATs) with hydrological streamflow models to provide a suite of stand-alone hydrology-land-surface schemes using SVATs as the common link; these stand-alone models are incorporated into atmospheric models to create a coupled system for operational forecasts (Pietroniro et al. 2007).

ECCC's GEM-Hydro is similar to MESH, but uses different land surface schemes (Gaborit et al. 2017). ECCC is implementing an upgrade to the land-surface schemes of the Global Environmental Multi-scale model (GEM), the Canadian national numerical weather prediction model (Gaborit et al. 2017). This new scheme assimilates space-based soil moisture observations and surface data, and simulates soil moisture and temperature (Gaborit et al. 2017). An evaluation of the capabilities of the new scheme from a hydrological point of view for streamflow prediction led to reasonable streamflow simulations for the Lake Ontario basin although some potential improvements were identified (e.g., a new snow module and surface ponding treatment) (Gaborit et al. 2017). GEM-Hydro can be used to estimate the Lake Ontario net basin supplies (the sum of lake tributary runoff, overlake precipitation, and overlake evaporation) (Gaborit et al. 2017). GEM-Hydro relies on a highly conceptual, 1D approach to groundwater as part of its river routing model. Weather forecasting does not require long-term trends in groundwater, so subsurface processes are represented by about a meter of the soil layer. Nevertheless, better understanding of longer temporal trends in groundwater may improve surface water modeling (V. Fortin, pers. comm. 2017). Model evaluations have been undertaken as part of the Great Lakes Runoff Intercomparison Project (GRIP), which seeks to better understand the status of existing model systems and to set a benchmark for model performance against which future models can be evaluated (Gaborit et al. 2017). A global calibration methodology was also assessed with respect to implementing hydrologic models over large areas and generating a spatio-temporally robust parameter set that can be transferred to nearby, ungauged areas (Gaborit et al. 2017).

ECCC's Water Cycle Prediction System (WCPS) is a chain of interconnected numerical models, coupling ECCC's atmospheric model (GEM), the surface and soil model Interactions between Surface–Biosphere–Atmosphere (ISBA), the lake/ocean model Nucleus for European Modeling of the Ocean (NEMO), the Community sea-ICE model (CICE), the river routing model WATROUTE for flow through the river network, and the Coordinated Great Lakes Regulation and Routing Model (CGLRRM) for flow through the lakes' interconnecting channels (Durnford et al. 2017). GEM-ISBA passes estimates of surface runoff and estimates of recharge from the soil column to WATROUTE (Durnford et al. 2017). The WCPS was implemented in June 2016 on the Great Lakes and St. Lawrence River by ECCC (V. Fortin, pers. comm. 2017). For the NEMO model, temperature conditions were taken from NOAA/GLERL's Great Lakes Surface Environmental Analysis (Dupont et al. 2012).

The US National Water Model (NWM) is a hydrologic model that simulates observed and forecast streamflow using mathematical representations of physical processes including snowmelt, infiltration and water movement through the soil layer (water.noaa.gov/about/nwm).

The model also provides forecasts of soil moisture, surface runoff and snow water equivalent. The NWM is run in four configurations: one-hour snapshot; short-range 15-hour deterministic forecast; medium-range ten-day deterministic forecast; long-range 30-day ensemble forecast (“The National Weather Model” 2017). The one-hour snapshots use USGS real-time streamflow observations to provide information on current streamflow and general hydrologic states. NOAA’s plans for the NWM include working with GLERL to model drainage into/from the Great Lakes; others have responsibility for levels of the lakes themselves (B. Cosgrove, pers. comm. 2017). The NWM uses the NoahMP Land Surface Model (LSM) to simulate land surface processes (“The National Weather Model” 2017). It currently takes a simplified approach to groundwater, treating it as a bucket and using empirical functions (B. Cosgrove, pers. comm. 2017). However, preliminary discussions have taken place with the USGS and the US Department of Energy to implement groundwater modeling; one goal consistent with NOAA’s hydrology mission is to forecast stream low flows (B. Cosgrove, pers. comm. 2017). Questions of computational feasibility and appropriate level of model fidelity have yet to be addressed (B. Cosgrove, pers. comm. 2017). No timeline has been established for this more advanced groundwater modeling work (B. Cosgrove, pers. comm. 2017). The USGS plans to leverage the NWM in an inter-agency program under development to produce national predictions of stream water temperature, erosion, and sediment/constituent entrainment and in-stream transport (S. Eberts, pers. comm. 2018).

The NWM is a particular instance of WRF-Hydro, configured to operate in NOAA’s weather services super-computing environment (B. Cosgrove, pers. comm. 2017). NCAR is the primary development partner with NOAA for WRF-Hydro (B. Cosgrove, pers. comm. 2017). WRF-Hydro offers a wide variety of options because it has the flexibility to turn on or off modules and to use more empirical approaches where desired (B. Cosgrove, pers. comm. 2017). WRF-Hydro has the capability to run high-resolution climate scenarios (D. Gronewold, pers. comm. 2017). If the computational needs get too large, the runs are done on a supercomputer accessible to NOAA (D. Gronewold, pers. comm. 2017). WRF-Hydro is being considered to address a need for modeling flood response predictions, which requires simulation of groundwater over relatively short timeframes (D. Gronewold, pers. comm. 2017). One particular challenge for future models will be to understand how groundwater fluxes will change over time with climate change (D. Gronewold, pers. comm. 2017). A recent study documents the coupling of HGS with the WRF for atmospheric, surface and subsurface integrated hydrologic simulation (Hamilton et al. 2018).

The North American Land Data Assimilation System (NLDAS) is developed by NOAA, NASA and several universities (B. Cosgrove, pers. comm, 2017). NLDAS is used within NOAA’s weather service to help initialize the weather models (B. Cosgrove, pers. comm, 2017). Two versions of the NLDAS-2 system are maintained: (1) an operational version to support operational analysis and prediction tasks; and, (2) a research and development version (Xia et al. 2012). NDLAS includes land surface models (LSMs) to simulate soil moisture, runoff, snow pack, and latent and sensible heat fluxes using atmospheric data points (e.g., precipitation, radiation, temperature, wind, humidity and pressure) that will forecast land surface states (Cosgrove et al. 2003). Four LSMs are used in NLDAS: Mosaic, Noah, Variable Infiltration Capacity (VIC), and Sacramento Soil Moisture Accounting (SAC) (Xia et al. 2016; Xia et al. 2012). NLDAS is similar to the NWM, but it is more focused on land surfaces (i.e., it does not simulate stream flows the way the NWM does) (B. Cosgrove, pers. comm, 2017). NLDAS has a longer-term retrospective dataset than the NWM (~15 years), although NWM’s dataset is growing each year (B. Cosgrove, pers. comm, 2017). NWM provides more results at higher resolution than NLDAS, but NLDAS offers more options for configuration and forcing products are readily available as inputs (B. Cosgrove, pers. comm, 2017).

The NOAA report, *Hydrological drivers of record-setting water level rise on Earth's largest lake system* (2016) (A D Gronewold et al. 2016) documents an analysis of the hydrological drivers contributing to the water level rise in 2013 and 2014 within the Great Lakes basin. Resulting estimates resolved the regional water budget across monthly and inter-annual time scales over a multiyear period for the Great Lakes (A D Gronewold et al. 2016). The results differentiate the hydrological, climatological, geological and anthropogenic drivers behind seasonal and long-term changes in Great Lakes water levels (A D Gronewold et al. 2016).

4.10 Fully-coupled groundwater-surface water models

Barthel and Banzhaf (2016) listed four fully coupled models most frequently identified in the literature globally that had been applied, or could be applied, at regional scales: ParFlow; HGS; InHM; and OpenGeoSys. MOD-HMS is also a fully-coupled model (Panday and Huyakorn, 2004). One advantage of fully coupled models is that they are run with one code, which can result in more stable results than running multiple models. A disadvantage of these models has been computational time; however, Aquanty Inc. has run HGS for large basins using advanced numerical methods and code parallelization (E.Sudicky pers. comm. 2018). Where long run times are needed for these models, the costs potentially preclude rigorous uncertainty analyses.

These types of models have a large number of estimated parameters and, where there is large uncertainty for boundary and initial conditions, formal calibration may be difficult (Fatichi et al. 2016). Note that other coupled model configurations also have numerous estimated parameters. As for any potential model configuration, uncertainty analyses require attention while recognizing the inherent limitations in uncertainty estimates. For fully coupled models, factors to consider include the advantages of complex physics, potential computational expense, ability to provide model inputs, and confidence in estimating parameters for regional scale models.

HydroGeoSphere (HGS) has been used in modeling studies for relatively small tributaries in Ontario within the Great Lakes basin: (1) the Duffins Creek watershed (286.6 km^2 or 111 square miles), a tributary to Lake Ontario (Li et al. 2008); (2) a 60 m (131 yard) stretch of Pine Creek, a tributary to Lake Huron (Brookfield et al. 2009); (3) Laurel Creek (17 km^2 or 6.56 square miles), a tributary to the Grand River flowing to Lake Erie (Sudicky et al. 2008). HGS was also used to estimate evapotranspiration in the Grand River Watershed (~7,000 km^2 or 2,703 square miles) and to develop an efficient calibration methodology for steady-state fully-coupled models (Hwang et al. 2015). Other HGS applications have been or are being developed in this scale range, for example a real-time hydrologic platform using the South Nation Watershed (~4000 km^2 or 1,544 square miles), a tributary to the Ottawa River/St. Lawrence system (E. Sudicky, pers. comm.2017) and in intermodel comparison studies.

On much larger spatial and temporal scales, a HGS model was built to simulate groundwater flow for Canada on a continental scale from the Wisconsin Episode glaciation to present (Lemieux et al. 2008). Key processes modelled included density dependent flow (i.e., brine), hydro-mechanical loading from the weight of the ice, subglacial infiltration and permafrost development (Lemieux et al. 2008). That model is being updated at a higher resolution and may provide boundary conditions for a Great Lakes basin prototype (E. Sudicky, pers. comm. 2017; see also Chen, 2015). The Geological Survey of Canada (in NRCan), the Ontario Geological Survey, and Aquanty Inc. are collaborating on the Southern Ontario Groundwater Project (2014-2019) (Frey, Berg and Sudicky, 2016) as proof of concept for a Great Lakes scale model (E. Sudicky, pers. comm. 2017). A study, *A feasibility study of merits and development strategies for* *a regional water resources modelling platform for Southern Ontario-Great Lakes* (2016) (Frey, Berg and Sudicky, 2016) includes a review of available datasets. The Great Lakes basin prototype will model transient but not steady state flows (E. Sudicky, pers. comm. 2017). Earlier versions of HGS did not handle precipitation as snow (AquaResource Inc 2011). HGS now has a module that can account for precipitation in the form of snow and the relationship of snowmelt with daily temperature and ground freezing or thawing (R. Therrien, pers. comm. 2017). A peer reviewed description of the snow module is in progress (R. Therrien, pers. comm. 2017). Aquanty is working with IBM to provide a front-end interface for users to use weather feeds from any forecast in the model (E. Sudicky, pers. comm.2017).

Inter-comparison studies have been undertaken to assess commonalities and differences among coupled surface-subsurface model results for test cases. A 2011 study commissioned by Ontario's Ministry of Natural Resources compared the capabilities and features of five models: HGS; ParFlow; MIKE SHE; GSFLOW; and MODHM (AquaResource Inc 2011). Three of these models (HGS, MIKE SHE and GSFLOW) were selected to simulate a water budget analysis for a headwaters subwatershed of the Credit River (a tributary to Lake Ontario) (AquaResource Inc 2011). Among these three models, MIKE SHE was selected to simulate a second subwatershed of the Credit River, the Mill Creek subwatershed, because it was the most flexible and user-friendly model code of the three models (AquaResource Inc 2011). A 2014 study of seven models based on benchmark problems included: HGS, ParFlow, CATHY, OpenGeoSys, PAWS, PIHM, and tRIBS+VEGGIE (Maxwell et al. 2014). All of the models simultaneously solve forms of the Richards and shallow water equations (Maxwell et al. 2014). In general, all models demonstrated the same qualitative behavior (Maxwell et al. 2014).

A second phase of inter-comparisons for three benchmark cases in 2017 included the models: HGS, ParFlow, CATHY, MIKE-SHE, GEOtop, ATS, and Cast3M (Kollet et al. 2017). Some models from the first phase were not included because they could not successfully undertake the benchmark tests in this phase (E. Sudicky, pers. comm. 2017). Overall the models agreed well in terms of temporal dynamics and hydrologic responses to heavy rain events, but exhibited differences in terms of absolute values for storage and discharge (Kollet et al. 2017). MIKE-SHE had a lower level of agreement with the other models for the subsurface storages (Kollet et al. 2017). There are plans to undertake a third inter-comparison study (E. Sudicky, pers. comm.2017). The USGS did not participate with GSFLOW in the inter-comparison studies of 2014 and 2017 because, as an entity that undertakes reimbursable projects within government, it does not typically undertake studies that have not generated stakeholder demand (and related funding) (S. Eberts and R. Hunt, pers. comm. 2017) and that are not clearly mission-focused (R. Niswonger, pers. comm. 2017). Also, the scale of the inter-comparison studies were on catchments that were much smaller than operationalized by the USGS in its studies (R. Niswonger, pers. comm. 2017).

A comparison of MODFLOW with HGS indicated advantages of using a code that can simulate both saturated and unsaturated flow and full coupling of physical groundwater-surface water processes for losing streams (Brunner et al. 2010). Note that in this comparison, the simpler RIV package was used for the MODFLOW configuration (Brunner et al. 2010) rather than the SFR2 package, which can simulate unsaturated flow beneath streams (R. Niswonger, pers. comm. 2017).

A 2016 study compared HGS, WATFLOW, MODFLOW and FEFLOW to delineate base flow contribution areas for streams in a southwestern Ontario watershed, Alder Creek (Chow et al.

2016). The models produced similar distributions of hydraulic head; however, capture zones differed and were sensitive to the particle tracking algorithm used (Chow et al. 2016). One study recommendation is that particle tracking and reverse transport delineation methods should be used together to improve confidence in predictions (Chow et al. 2016).

A new set of models is being developed under the US Department of Energy Accelerated Climate Modeling for Energy (ACME) project with planned flexibility (e.g., options for grid, mesh, 3D, 2D, 1D) and coupled heat and moisture transport and 3D formulation of Richards Equation; the model will be publicly available (V. Ivanov, pers. comm. 2017). According to an ACME brochure, the model

> "…simulates the fully coupled climate system at high-resolution (15-25km) and will include coupling with energy systems, with focus on a near-term hindcast (1970-2015) for model validation and a near-term projection (2015-2050) most relevant to societal planning. The model further employs regional-refinement using advanced adaptive mesh methodologies in order to provide ultra-high-resolution to resolve critical physics and meteorological phenomena.[5]"

There are three initial scientific goals, including investigating how the water cycle and water resources interact with the climate system on local to global scales. This research includes shorter term (three-year) simulations to assess climate interactions with freshwater supplies and longer term (ten-year) simulations of interactions of water, climate and forcing agents such as aerosols and greenhouse gases. The other two goals pertain to biogeochemical cycles and cryosphere-ocean system interactions.

4.11 Other supporting modeling tools

Several additional tools and methods for assessing model results or for calibration were identified in the literature and by researchers who were contacted.

Gravity Recovery and Climate Experiment (GRACE)

Satellite data gathered through the GRACE mission are capable of detecting changes in total water storage (TWS) by measuring Earth's gravity field anomalies (Yassin et al. 2017). GRACE can be applied to estimate changes in TWS across large watershed systems but cannot estimate absolute TWS (Huang et al. 2012). The dataset has the potential to serve as a comparison with other modeling results; however, GRACE data are challenging due to coarse spatiotemporal resolution, several sources of uncertainty (Yassin et al. 2017), and the requirement for specialized expertise.

Geological weighing lysimeters (GWLs)

Natural lysimeters may be useful for testing and improving parameterizations and model structures used for hydrological simulations or in regional or global atmospheric models (Marin et al. 2010). WATFLOOD water balance results were assessed using a confined aquifer as a geological weighing lysimeters (GWL) for a study area of 314 km^2 (121 square miles) in Saskatchewan with suitable climatic conditions (Marin et al. 2010). Further analyses and modeling of confined aquifers as GWLs are needed since the magnitude of the water storage

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[5] ACME Overview Brochure, retrieved Feb 2018 at https://climatemodeling.science.energy.gov/sites/default/files/publications/ACME_Overview_Brochure_3.pdf.

changes and extent of the area represented were not precisely defined in this study (Marin et al. 2010).

Metamodels

Metamodels are a statistical approach to understanding a range of outputs from numerical models, developed to overcome long runtimes for sensitivity analysis of complex models (Fienen et al. 2015). A statistical technique, such as Bayesian networks, artificial neural networks, or regression trees, is selected to develop a predictive model “learned” from relationships among the process models’ inputs and outputs (Fienen et al. 2015). The resulting metamodel can be incorporated into a decision-making framework to gain quicker insights to conditions than offered by complex models, while recognizing the metamodel predictions have lost some precision (Fienen et al. 2015). Metamodels are a complementary approach, not an alternative to complex model development (J. Starn, pers. comm. 2017). In an application mentioned above, the USGS applied metamodeling techniques to assess streamflow balance and potential depletion in response to shallow well pumping (Feinstein et al. 2016); predictions included uncertainty estimation and extended to depletion potentially beyond the modeled area. Further, the USGS evaluated three metamodeling techniques using the MODFLOW-USG model (Feinstein, Hunt, and Reeves 2010) of the Lake Michigan basin, specifically to assess their utility in providing stream-depletion information to potentially augment decision support for permit applications to extract groundwater (Fienen, Nolan, and Feinstein 2016). In that study, the characteristics and performance of three techniques were compared: Bayesian networks, Artificial neural networks, and Gradient Boosted Regression Trees (Fienen, Nolan, and Feinstein 2016). The study results indicate that a metamodel has the potential to provide predictions over a larger spatial range than the regional numerical model to which it is fit (Fienen, Nolan, and Feinstein 2016). At the time of writing this report, a project is planned to develop a metamodel using the results of MODFLOW models applied to glaciated aquifers across the US (J. Starn, pers. comm. 2017). The USGS also has two publications pending on the use of metamodels in groundwater age calculations[6] (D. Feinstein, pers. comm. 2018).

Parameter estimation (PEST)

PEST (Parameter ESTimation) is a program to adjust parameters to fit model outputs to a set of observations as closely as possible (Doherty 2002). This functionality assists in data interpretation, model calibration and predictive analysis (Doherty 2002). Where non-unique parameters are identified, PEST provides an analysis of the implications for predictions made by the model (Doherty 2002). PEST is a nonlinear parameter estimator and it runs the model as many times as necessary to identify an optimal set of parameters (Doherty 2002). PEST requires that upper and lower bounds for adjustable parameters be identified so that it will operate within the permissible range of values for these parameters (Doherty 2002). PEST was used extensively in literature identified in this review.

4.12 Key Data Gaps

There was no clear consensus among the scientists interviewed on the most important data gaps, or that critical gaps exist. One potential explanation for these varied views is the very

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[6] Feinstein, D.T., Kauffman, L.J., Haserodt, M.J., Clark, B.R., and Juckem, P.F., Extraction and development of inset models in support of groundwater age calculations for glacial aquifers: U.S. Geological Survey Scientific Investigations Report 2018, in press.

Michael N. Fienen, B. Thomas Nolan, Leon J. Kaufman, Daniel T. Feinstein, "Metamodeling for Groundwater Age Forecasting in the Lake Michigan Basin". submitted to Water Resources Research, in review.

preliminary state of the discussion about a model. Without knowing the key expectations, scale or scope of a model, the level of data detail required is unknown. Opinions stated by scientists are not attributed in the following discussion.

One scientist indicated that more data could always be used but data gaps do not present an insurmountable problem. Another stated that there is unprecedented ability to do a first cut model given comprehensive geographically referenced datasets. However, others expressed concerns about not having sufficient real data for groundwater model validation. Some concerns were also expressed about datasets that are dispersed among many jurisdictions and organizations within jurisdictions, making access problematic and integration a huge task. For instance, borehole logs, digital elevation models, and other data are not managed centrally in some jurisdictions and, in some cases, private data held in public databases are not accessible due to economic factors and/or confidentiality considerations (e.g., decreased property values or proprietary corporate information). Data for precipitation, recharge and levels of lakes are very detailed and available, although with geographically inconsistent density of gauges in the basin. North of Lake Superior there is sparse monitoring coverage whereas in other areas, such as the Toronto vicinity and in the Michigan basin, there are very dense monitoring networks. A couple of scientists expressed concern over the state of groundwater use data in Canada but another indicated that missing groundwater use data can be compensated for with inferred values from population and agriculture statistics. There are inconsistencies in subsurface information from state to state in the United States, as well as the US-Canada cross border.

A preliminary investigation of data availability to develop a fully coupled model (using HGS) for the Great Lakes basin and southern Ontario identified a need to improve the uniformity of the Canadian hydro-stratigraphic characterization within the subsurface sedimentary layers with that for the United States side of the basin (Frey, Berg and Sudicky, 2016). Also, inference of hydraulic properties of the subsurface materials, specifically sedimentary and crystalline rock formations, cannot be made based on current information (Frey, Berg and Sudicky, 2016). The United States has information on vertical gradients for hydrologic conductivity for multiple layers but this information is lacking in Canada. The US methods used to develop a hydrogeologic framework for glacial aquifer systems (Reeves et al. 2017) may be applicable for Canadian development of this data. Further information will be available from the USGS when a compilation of digital maps and report are published later in 2018; this compilation, *Hydrogeologic Framework for Characterization and Occurrence of Confined and Unconfined Aquifers in Quaternary Sediments of the Glaciated, Conterminous United States: A Digital Map Compilation and Database*, is in final editorial review (S. Eberts, pers. comm., 2018). Cross-border areas can present challenges where geologic mapping information does not necessarily agree at adjacent or overlapping geographic regions (Brodaric 2012).

Surface and near surface (i.e., soils) data are readily available (Frey, Berg and Sudicky, 2016) but others indicated that, on a basin scale, surface soil texture data were sparse other than for agricultural lands; urban areas are a particular gap in soils and surface data. Glacial deposits are very simplified in models within the basin due to the deglaciation process that resulted in very heterogeneous deposits, including localized thick gravel deposits and clay marine deposits. LIDAR can readily map surface data but that technology does not reveal third dimension characteristics below the surface. There are discontinuities between the United States and Canada in terms of detailed representation of soil moisture and soil temperature on a basin scale. Specifically, data resolution in Canada is low, with little information on soil texture, and data are not reported in the same way as it is in the United States (e.g., Canada uses different soil categories and different representation in the vertical direction). There are global databases for soil texture but they have low resolution. Land surface vegetation information may not be available at sufficient resolution for atmospheric model use, especially in northern Ontario where the interactions of soil with vegetation under cold climate conditions are often poorly represented.

The Great Lakes Aquatic Habitat Framework (GLAHF) project has developed some basinwide resources (C. Riseng, pers. comm, 2018). For instance, a recent study by Wang et al (2015) developed a spatial classification framework and database. Catchments in the database have been attributed with physicochemical and biological characteristics of the lakes using spatial classification zones (coastal terrestrial, coastal margin, nearshore and offshore zones) (Wang et al. 2015). This spatially structured database is intended for use in development of basinwide management plans and other studies or research (Wang et al. 2015). Another recent report by Forsyth et al (2016) identified consistent binational watersheds for the entire basin. One product of this study is the Great Lakes Hydrography Dataset (GLHD), consisting of 5,589 watersheds based on flow direction grids that have been hydrologically vetted by government water resource agencies (Forsyth et al. 2016). The GLHD is a publically available geodatabase (Forsyth et al. 2016) accessible at glahf.org (C. Riseng, pers. comm, 2018). NOAA has accessed data from the GLAHF for development of WRF-Hydro (C. Riseng, pers. comm, 2018).

A gap of particular relevance for coupled models is the limited quality and abundance of field data for hydraulic head in aquifers and data to represent streambed heterogeneity in models[7]. In general, there is limited understanding of the appropriate level of complexity to model processes, scale and heterogeneity (Frey, Berg and Sudicky, 2016; Bierkens et al. 2015) and thus the range of data needed to support the inter-relationship of aquifer hydraulic head and stream beds is not known. Representation of the interaction of vegetation and soil (and therefore groundwater-surface water relationships) is especially challenging in northern Ontario, in part due to cold conditions. For the RASA model of groundwater of the Michigan peninsula (circa 2000), convergence issues identified during calibration may have been the result of a disconnect between the head and flow data, specifically 30-year steady-state base flow data mixed with scale- and time-dependent head data (Hoaglund, Huffman and Grannemann, 2002).

The Canadian Groundwater Information Network (GIN) houses groundwater information from participating jurisdictions (including Ontario). The GIN dataset was created to gather, in the same dataset, all available data and information for all aquifers, aquifer systems and hydrogeological contexts of a project. GIN provides: a) a Canadian national framework for connecting groundwater information; b) web access to groundwater data via the GIN Portal; c) standards for exchanging data; and, d) analysis and modeling tools (GIN website). GIN provides access to water well databases, water monitoring data, aquifer and geology maps, and related publications. Collaboration with the USGS is underway to enable cross-border sharing of similar groundwater information; GIN is aligned with USGS standards. The Geological Survey of Canada is working on a pilot project to enhance access to information on data linkages by documenting the relationships between key features (B. Brodairic, pers. comm. 2017). For instance, the pilot will provide information on the linkage between stream gauges, a stream of interest, and a nearby aquifer without the need to download datasets and GIS mapping. Similarly, the USGS Geospatial Fabric for the US national hydrologic modeling initiative includes two main products: 1) GIS features and 2) tables of attributes about those features.[7]

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[7] USGS Geospatial Fabric website at URL: https://wwwbrr.cr.usgs.gov/projects/SW_MoWS/GeospatialFabric.html, accessed February 2018.

The issues of data availability or gaps extend beyond the data themselves. For a living GW-SW model, a responsible agency must acquire and maintain a database that includes both static information (e.g., subsurface layers) and dynamic information (e.g., flow rates, variation in groundwater levels, land use, etc.). Note that even the 'static' data on subsurface layers needs to be maintained to incorporate new data and/or new interpretations over time. Access to a model that is calibrated and continually improved, provides a tool that can be used to integrate and interpret monitoring data, setting up a positive feedback loop for improved modeling capabilities. Assimilation of data on the scale of the Great Lakes basin to support a GW-SW model presents model optimization and data assimilation challenges, in addition to considerable computational demands.

For atmospheric models, climate change represents a significant challenge for downscaling models and modeling methodologies. A two-year Canadian project just getting underway will assess the applicability of the approach to weather forecasting (lake hydrology coupled with atmosphere) for better climate change predictions than offered by current climate change models (V.Fortin, pers. comm.2017).

Potential sources of data in the United States are numerous and include: the USGS seamless data viewer (http://nationalmap.gov/viewer.html), the National Resources Conservation Service web soil survey (http://websoilsurvey.sc.egov.usda.gov/App/HomePage.htm); precipitation data from multiple platforms are available from the National Center for Environmental Information (formerly the National Climatic Data Center, http://www.ncdc.noaa.-gov/); meteorological forcings from NALDAS (http://www.emc.ncep.noaa.gov/mmb/nldas/) (Fatichi et al. 2016). The USGS provides real-time streamflow observations.

ECCC also provides streamflow data. The USGS also makes available estimates of monthly water yields and flows for the US portion of the Great Lakes basin in a web-based mapper application, along with monthly flow time series for individual stream segments (Luukkonen et al. 2015) available from 1951 to 2012 (H. Reeves, pers. comm, 2018). In addition, as of October 2016, all USGS model input/output files and calibration data are published online with the accompanying USGS modeling report (S. Eberts, pers. comm, 2018). Files are available via the USGS Science Data Catalog; groundwater models are tagged with "USGSgroundwatermodel" (S. Eberts, pers. comm, 2018). The Geological Survey of Canada is developing a 3D stratigraphic model for southern Ontario (B. Brodaric, pers. comm. 2017) to serve as the foundation for computer simulation of water flows. The model is being built using LEAPFROG, a geological model package (B. Brodaric, pers. comm. 2017). There is a binational (US-Canada) nutrient model under development for the Great Lakes basin and other shared watersheds, as part of a coordinated project by the USGS, the National Research Council of Canada, and the IJC. The SPARROW (*SPAtially Referenced Regressions On Watershed* attributes) models track nutrient transport, with a focus on nitrogen and phosphorus from local to regional watershed scales and to coastal waters by analyzing spatial water quality patterns, human activities, and natural processes.[8]

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[8] USGS SPARROW website at URL: https://www.usgs.gov/centers/wisconsin-water-science-center/science/sparrow-watershed-modeling-binational-uscanada-models?qt-science_center_objects=0#qt-science_center_objects, accessed February, 2018.

5 Potential approaches

5.1 Receptivity to a GW-SW model for the basin

Scientists interviewed in this project support improving the scientific understanding of the water balance at the basin scale in the Great Lakes basin. Specifically, they support improving understanding of the role and importance of groundwater in the water balance. The scientists also considered that an accessible basin-scale model would be a valuable asset because it could provide boundary conditions for more regional or local-scale models.

Confidence varied among the scientists with respect to the current capabilities of modeling options to successfully develop, calibrate and run a basin-scale groundwater-surface water model. Reasons for lower confidence included: uneven data availability across the basin; high computational loads that might limit the calibration and sensitivity analyses for the model; limited scientific knowledge of scaling requirements to move from local to basin scales; and limited confidence in modeling options given the high parameterization and low knowledge of initial conditions.

5.2 Potential approaches

The following four approaches present potential approaches for the first phase of work. They are not necessarily mutually exclusive. For instance, option 1 may precede either option 2 or option 3. Similarly, option 2 may precede option 3.

1. Focus on data assembly, building data sharing protocols, and developing a shared conceptual transboundary model

The premise underlying this approach is two-fold. First, the database is ultimately the product with the highest value over the long term. Various modeling platforms and codes will be developed and applied over the years but assembly of a high quality, shared database will underpin all modeling efforts at the basin scale, as well as more regional/local scales.Second, a harmonized hydrologic conceptual model is needed under any modeling approach that is selected.

Further rationale for this approach is that several groups are currently assessing the addition of more advanced treatment of GW-SW interactions into their modeling platforms. This includes: The Global Water Futures project (University of Saskatchewan, University of Waterloo, ECCC); NOAA/NCAR/US Department of Energy for WRF-Hydro and NOAA/NCAR for the NWM, along with USGS for linkages to the NWM; Geological Survey of Canada, with the Ontario Government and Aquanty Inc. for southern Ontario.

In this option, the IJC is more engaged in process development than in scientific research or model development. The IJC's work to support data assembly would run in parallel with the work by others to research modeling methods for GW-SW interactions.

Similar to the IJC's data harmonization initiative for drainage basins, the IJC could extend its harmonization work to subsurface systems. A hydrologic conceptual model for the surface-subsurface system could then be developed. Although this conceptual model would include both surface and subsurface elements, the process could be informed by experience gained during the development of a subsurface conceptual model for the Milk River (Pétré et al. 2016). The IJC could also provide oversight for various agreements to reproduce science and share data, including: data access; standards and protocols for categorization and nomenclature of transboundary subsurface features; quality control protocols; and procedures for incorporation of new data as it becomes available. This process and related protocols will enable modelers from a range of stakeholders to access the database for a basin scale and other modeling initiatives. As part of this process, key data needs may need to be identified and prioritized in collaboration with the researchers identified above.

Pros for Approach 1:

- The harmonization and protocols could be extended to include the St. Lawrence watershed, so that the entire drainage basin has a seamless approach to data access and storage.

Cons for Approach 1:

- Not all data are needed or useful for basin-scale modeling; effort spent on protocols, data acquisition and/or incorporation into a database for data may beuseful only at local scales.
    - ➢ To mitigate this risk, IJC could work in close collaboration with organizations undertaking research on scaling up GW-SW processes from local to regional or basin scales.
- Lack of open access to databases and models developed by others (e.g., through academic research).
- Delays the IJC initiative for basin-scale modeling.
- Sustaining organizational commitment and funding for database development and maintenance can be challenging if data analyses/reports are not also produced to demonstrate a need for the database.

2. Build individual, simplified models for groundwater and surface water on a basin scale to assess data gaps and calibration issues

This approach develops a groundwater model on a basin scale and models surface water on a basin scale to draw preliminary conclusions. The premise underlying this approach is that building individual, simplified models is the best way to discover key data gaps, to assess the need and viability of more advanced models, and to assess issues to be addressed if more complex modeling efforts are deemed necessary. Another rationale for this approach is that the trends and magnitude of GW-SW interactions at a basin scale are unknown; improved scientific understanding is needed but the appropriate level of effort to allocate to modeling is unknown, given that the interaction may not be significant on a basin scale.

With respect to modeling effort, an initial, simplified approach to modeling can inform the model design. A couple of initial large cross-sectional models and a simple 2D or 3D subsurface model may answer key questions before coupling models together (R. Lefebvre, pers. comm. 2017). Starting with a 2D coarsely gridded model would allow assessment of the sensitivity to changes (J. Starn, pers. comm. 2017). At the basin scale for the Great Lakes, the subsurface aquifer is relatively thin and the dominant direction of flow is horizontal, raising the possibility that a simplified 2D groundwater model could be used for the initial analyses (R. Hunt, pers. comm. 2017). Other preliminary design questions that could be informed by this approach include: What thickness of subsurface system needs to be considered? Is interbasin groundwater flow of sufficient magnitude to warrant basinwide modeling with advanced models? How fine do grid cell sizes need to be for meaningful results? What is the computational burden of the minimum grid cell size on a basin scale? Do the computational requirements preclude use of grid cell sizes that provide useful results? Does the minimum grid cell size offer the potential to provide boundary conditions for regional or local-scale modeling for specific studies? Information from this initiative would also inform data prioritization to fill gaps in preparation for more sophisticated models if needed.

This approach is consistent with the view of some scientists interviewed that it is better to run a model early and find holes in the data through the model rather than look for data up front. In order to make resource allocation decisions, it would be useful to have a preliminary assessment of the magnitude, relative to uncertainties, of GW-SW interactions at a basin scale. The work plan would include quantification of uncertainty associated with the first level of modeling to assess at what point decisions can be made in a cost-effective fashion *vis a vis* model development effort. This approach also is consistent with a commitment to iteration in model development. In recognition that software evolves, an early iteration based on available data and codes provides insights to top priorities for data collection, research and modeling capabilities and helps set an agenda for further refinement as science and code advance.

Models selected under this approach could include groundwater models, surface water models, and models that take a simplified approach to one of these components (e.g., atmospheric models that use LSMs with simplified groundwater assumptions).

Pros for Approach 2:

- Provides insights to the role of groundwater and surface water on a basin level in advance of more sophisticated modeling efforts.
- Quickly identifies significant data gaps in both surface water and groundwater domains and informs data collection and coordination efforts in terms of key gaps and monitoring needs.
- There is a large pool of modeling experts and many options for selection of model codes to use.
- May improve understanding of the water balance on a basin scale.
- Opens the potential for several models to be developed for comparison and discussion because there are more researchers with experience and expertise in either groundwater or surface water model codes (both proprietary and open source) than in fully integrated codes. A large pool of experts allows for intercomparison studies to assess model performance.

Cons for Approach 2:

- Convergence problems may result wherein the results of two independently developed models do not agree and cannot be resolved without considerable additional effort.
  - ➢ The impact of this risk may be minimal if the primary goal of the modeling exercises is to identify key data gaps.
- If an integrated model is needed, there may be some lost effort in developing individual models first.
- The individual preliminary models may be limited in terms of their usefulness to set boundary conditions for regional or local inset modeling.

3. Build an iteratively-coupled model on a basin scale

This approach is similar to Approach 2 except it includes an intention to iterate the output from a groundwater model with that of a surface water model. The rationale for this approach is that the iteration process would provide some insight to GW-SW interactions while allowing for development of basin-scale groundwater and surface water models. This approach likely limits the model selection to only those codes that have demonstrated their applicability and performance within an iteratively coupled model scheme. MODFLOW would likely be a frontrunner for a groundwater model under this scenario since it has been used on smaller scales within the basin already; it has also been used within an iteratively coupled configuration (e.g., with PRMS).

Pros for Approach 3:

- Provides insights into the role of interactions on a basin level.
- Identifies significant data gaps in surface water and groundwater domains and informs data collection and coordination efforts in terms of key gaps and monitoring needs.
- Likely to improve understanding of the water balance on a basin scale.

Cons for Approach 3:

- Convergence problems may still result, similar to Approach 2.
  - ➢ This risk could be mitigated by an experienced modeling team and selection of modeling platforms.
- The requirement for iteration limits the flexibility offered by Approach 2 where two independent models can be developed by various groups; modeling team(s) with experience in both surface and groundwater modeling will be needed.

4. Build a fully-coupled groundwater-surface water model on a basin scale

This approach entails a commitment upfront to a fully coupled GW-SW modeling platform. As a preliminary step in this process, a simplified model could be developed using the selected fully coupled platform, and is a normal part of model development (E. Sudicky, pers. comm. 2017). However, the clear intention of this approach would be to develop a model that provides a simultaneous solution of process-based equations with 3D subsurface representation. The premise of this approach is that these models and associated methods for calibration and sensitivity analyses offer the best solutions to GW-SW interaction questions. It must also be assumed that the models and methods will produce meaningful results on a basin scale and that the computational burden of this approach can be addressed through cloud computing or other suitable approaches.

There is some debate within the scientific community about the ability to run uncertainty analyses for these models due to the large number of parameters and the associated computational burden. There is also debate with respect to the value of a deterministic model for GW-SW interactions, especially considering the limited knowledge of initial conditions (e.g., soil conditions). There is a requirement for very good documentation of the choices made to constrain the model to produce parameters and for the rationale that has led to those parameters being considered reasonable.

Pros for Approach 4:

- The simultaneous solution of process-based equations is scientifically advanced.
- Saves preliminary effort on other options if a fully coupled model is needed.
- Similar to Approaches 2 and 3, this approach is consistent with the philosophy of getting a model underway earlier rather than organizing data first.
- If a 3D model is crucial for modeling Great Lakes processes for water quality in the future, this approach commits early to adopting a model with this capability.

Cons for Approach 4:

- May take more time to get preliminary results than for Approaches 2 or 3.
- Smaller pool of experts to draw on for modeling expertise.
    - ➢ This limitation may be short-term if these models become more extensively applied and as Cloud computing options develop.
- Fewer agencies have this type of model code, so reduced accessibility to run scenarios or for use to set boundary conditions in future work.
- May require an ongoing commitment to specialized resources to maintain and use the model (depending on licensing and training options).
- Fully coupled models may have to be scaled down to provide useful answers, in the same way global climate models need to be scaled down to model local climate change forecasts; there are challenges in scaling up or scaling down.
    - ➢ This risk could be mitigated by development of submodels at multiple scales to understand the limitations related to a basin scale model.

6 Workshop discussion

6.1 Workshop overview and objectives

A two-day workshop was held in Ann Arbor, Michigan, on April 4-5, 2018. Over 40 people participated in the workshop from various organizations located in Canada and in the United States. There were participants from several universities and nongovernmental organizations as well as government agencies, including the USGS, Geological Survey of Canada, NOAA, ECCC, provincial and state governments. A list of participants is provided in Appendix B.

The workshop convened a group of experts to provide input for consideration by the IJC in order to:

1. Select and develop a modeling approach to assess the water balance of the Great Lakes basin, at the basin scale, through combined representation of surface and subsurface hydrological processes;
2. Understand the gaps and limitations associated with various options for a modeling approach; and,
3. Understand the implications of modeling choice for future work on water quality and ecosystem health.

The workshop consisted of a mix of formal presentations, panel discussions, breakout group sessions and plenary discussions. The workshop agenda can be found in Appendix C, along with the reporting sheets from the breakout sessions. A deliberate feature of this workshop was its flexible agenda. The first day included a number of presentations and panel discussions intended to set the stage and identify the topics and need for further discussion. The final breakout group discussions at the end of the first day determined the specific issues and topics discussed on the second day. The workshop organizers and facilitators analyzed the reporting sheets from the breakout session during the evening and used this input from participants to set the agenda for the second day.

6.2 Specific themes and questions for discussion

The workshop was planned around three themes:

1. Modeling approach;
2. Data needs and gaps;
3. Future applications.

The following questions were developed in advance of the workshop and distributed to participants to inspire additional questions and issues for discussion during the workshop.

Modeling Approach

- Is it feasible to model GW-SW interactions at the basin scale for the Great Lakes basin?
- What are the strengths and gaps for each of the potential modeling approaches?
- Does a commitment to the model approach need to be made within a terms of reference (TOR) to proceed with the work (e.g., individual models for GW and SW, loosely coupled[9] or fully coupled)?
- What core elements should be included in a TOR for a proposal call to model groundwater-surface water at the basin scale?
- Are there modeling approaches that preclude estimates of uncertainty (due to limited science, computational demand, limited statistical methods, other)?

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[9] The term loosely coupled is maintained here because that was the wording used in the workshop question.

- What requirements should be included as part of a groundwater-surface water model "contract" to estimate uncertainty associated with model results?

Data needs and gaps

- In developing a model for the basin scale to assess the contribution of groundwater to the water balance, what data are required that are not currently available?
- What techniques (if any) can be used to fill these data gaps assuming the data will not be available at the start of the project?
- What are the current issues in data harmonization and what can be done to address them?
- From the perspective of hydrogeology, how many subsurface layers is reasonable or feasible at a basin scale?

Future applications

The first priority for model results is to understand the water balance at the basin scale. Examples of future applications may include questions about water quality, low flow conditions, ecosystem health issues (e.g., habitat quality), climate change scenarios, and resource extraction implications.

- How can flexibility for future applications be maximized during development of the water balance model?
- What gaps would be left by each of the modeling options or by the selection of particular model platforms?
- Are there modeling approaches that preclude development of predictions for various future applications?

6.3 Key Outcomes

Vision for the model

All workshop participants agreed, at a conceptual level, that a basin-scale model would be beneficial to better understand GW-SW interactions on a Great Lakes basin scale.

Suggestions and discussion to develop a vision for the model further included:

a) Identify and consult with stakeholders to identify needs that could be met with a basin-scale model, and to build a broad base of support for developing such a model;
b) Identify questions important to the integrity of the Great Lakes-St. Lawrence River Basin Water Resources Compact, including projected future groundwater withdrawals, nutrient flows in GW/SW and potential low flow conditions, which should be considered during model development;
c) Develop a shared, unified model and/or modeling approach and/or model framework for use by both Canada and the United States to increase opportunities to build unified approaches and to avoid conflict;
d) Keep in mind multiple scales, from local to regional to basinwide, so the basin-scale model and/or model framework provides boundary conditions/context for other studies on smaller scales.

Advocacy for GW-SW modeling by the IJC and its boards would assist in building support and engagement. Other IJC initiatives, such as data harmonization, have successfully garnered support and leveraged talent in both countries.

Modeling Approach

It was generally agreed that no single model should be selected at the outset for use by all agencies and researchers to assess water balance on a basin scale. It was also generally agreed that modeling a complex system such as GW-SW interactions on a basin scale requires a step-wise approach, starting with simplified constructs before moving to more detailed representations. Deconstruction of the problem and a vision for the model were identified as key to any successful modeling initiative. Several ideas were discussed with respect to how to approach an initiative to develop basin-scale GW-SW models, including:

a) The first step, as identified by workshop attendees, is to develop a shared conceptual model of the Great Lakes basin hydrologic system. Publication of this basinwide hydrologic conceptual model was recommended so it can be cited in future modeling work. A precedent for this work, albeit smaller in scope and limited to subsurface features, is the hydrogeological conceptual model of the Milk River transboundary aquifer (Pétré et al. 2016).

b) A second group of priority activities pertain to data availability and use, including data sharing plans and agreements and data harmonization. Stakeholder input is needed to understand their needs, potential contributions of data and expertise, and to assess the appropriate scale(s) for modeling. A specific need to harmonize subsurface information, including nomenclature for subsurface features, was identified.

c) Many participants felt the IJC and/or agencies with modeling capacities should develop a basin-scale framework that brings together data and information needed to conduct basinwide hydrologic investigations. A framework would also guide stakeholder engagement and foster inter-agency collaboration. Data sharing plans and agreements and data harmonization (mentioned above as a second priority) would be part of the framework. Initially, the framework would not necessarily include a numerical model, but any basin-scale numerical model or models would eventually be part of the framework. The framework (and eventually the numerical model(s)) would support stakeholders in smaller-scale investigations and would facilitate nesting of models.

d) Model inter-comparison studies will be important and should be carefully designed. Protocols and implementation strategies analogous to those used by the IPCC to improve atmospheric/climate change models were suggested. This approach requires identification of forcing data and metrics for assessing results. The end points for modeling will influence the models used (e.g., lake levels versus nutrient exchange).

e) There was general agreement on the benefits of undertaking pilot studies to help scope any basinwide numerical modeling:

    i. Opportunistic studies using off-the-shelf products to demonstrate the potential to scale-up and/or collaborate across borders/disciplines/agencies; these opportunities would require minimal funding and rely on in-kind support and possibly post-doctoral or graduate student support.

    ii. Formal studies with sufficient funding to demonstrate the applicability of one or more model code options with the intention to scale-up to basin scale and further develop the pilot model into a basin-scale tool.

Opportunistic studies may get underway in advance of formal inter-comparison studies as proof of concept and/or to build working relationships. However, the second group of formal pilot studies should be undertaken within the context of model inter-comparison protocols.

f) Basinwide numerical modeling should begin simply to determine appropriate vertical and longitudinal scales. This approach would provide an understanding of inter-lake groundwater flows and the geographic range for groundwater transport within the system (or, as one attendee stated, to find out whether the lake system is a bathtub or an egg carton). Applications of complex and simplified models are not mutually exclusive; paired modeling approaches can be used, depending on the question. Uncertainties arise with both simple and complex models so both structural and other sources of uncertainty must be characterized to the extent possible.

Data needs and gaps

The discussion regarding data needs was wide-ranging, reflecting various interpretations of the model vision, key questions and potential future applications. There was general agreement that modeling would be feasible with available data if the question(s) were well defined and the uncertainties associated with data gaps and scientific limitations were stated as part of any modeling study. Data support needed for modeling will be dependent on the scale of model implemented and the questions asked. The need for a strategy on data collection was identified, including where and how often to gather data, and reflecting the needs of the question (e.g., operational functions requiring real time data versus scientific research questions).

While no participants were cautioning against model development until more data are available, in general, there are few robust harmonized datasets to feed into a basin-scale model. However, ongoing research will add new datasets such as the Global Water Futures research project (a consortium led by the University of Saskatchewan). Some specific data gaps were identified, including:

a) A missing integrated view of the hydrological budget for the Great Lakes, including understanding how frozen ground affects water cycling and the precision needed to represent vast areas of wetlands in a basin-scale model.

b) Data availability and depiction of subsurface geology for groundwater modeling.

c) Availability of reliable rainfall data that is subject to quality control protocols.

d) A need to agree on a forcing dataset for a systematic approach to forcing models (e.g., for comparison and trend analysis).

e) A need to gather, collate and verify the dispersed data from water wells and driller records. The database developed by the Toronto and Region Conservation Authority, initially to house data on the Oak Ridges Moraine, may provide a template for this type of database.

f) Data collection for groundwater will be different than for surface water; there is a need to identify the scale effects of groundwater and resolve its compatibility with surface water data scales.

Future applications

A range of future applications was discussed throughout the workshop. The themes for future applications broadly pertained to supporting management, resilience and sustainability of the ecosystem and resource use. Some specific modeling applications identified include:

a) Groundwater contribution to lake-level fluctuations and water balance
  - An example of a practical application of this information is to predict lake level changes. The IJC is expected by stakeholders (governments and citizens) to explain changes to water levels and to make predictions about what changes may occur in the future. Issues range from navigation to dock maintenance to property damage from flooding.

b) Nutrient loading and pathways
  - Including stream flow depletion and nutrient mass transport.

c) Climate change effects on water temperature and environmental flows. For instance, potential study topics include:
  - The seasonality of precipitation changes, shifts in the timing of the pulse of groundwater to the Great Lakes and effects of non-stationarity of the hydrologic cycle;
  - Runoff versus recharge and long-term climate trends on atmospheric/surface energy fluxes (influencing drought for example);
  - The relationship of temperature with groundwater-surface water interactions;
  - Climate change effects on low flow levels, habitat, ecology.

d) Water availability, suitability, and sustainability for agricultural use, drinking water, industrial use, and ecosystem function. Specific issues identified include:
  - Anthropogenic water demand and changes in the groundwater boundary to the Great Lakes;
  - Aggregate dewatering effects.

e) Floodplain function and management
  - Including the contribution of groundwater flooding to flood events.

Challenges and outstanding issues

Several outstanding issues pertaining to an initiative to model GW-SW on a basin scale were identified, including:

a) Is the model (are the models) operational or science-based (i.e., intended for research)? What agency/agencies will run it/them? Is there a role for non-government organizations?
b) Models need budgets and other resources to stay ‘alive’; identifying agencies that are mandated to answer the questions posed will be important for sustained support for modeling on a basin scale;
c) Political challenges to having eight states and two provinces agree on a common reporting and data systems. IJC may play a role in facilitating this coordination;
d) The U.S. Department of Energy is working on a comprehensive model that includes the water cycle but limited information was available prior to the workshop.

7 Recommendations

7.1 Development of an integrated GW-SW model

Integrated GS-SW modeling to understand changes in net groundwater storage and other water balance components at the basin scale for the Great Lakes basin has good support among expert scientists. Modeling to understand the water balance more fully has the potential to support a wide range of future applications; however, the future applications supported will depend on the specific design questions and the models that are developed in response.

Modeling at this scale in the Great Lakes basin is considered feasible, although it will benefit from collaborative efforts by agencies in Canada and the United States on management and scientific/technical issues. The management and scientific/technical threads are not mutually independent; each will support the advancement of the other.

Management Collaboration

A management framework for the initiative should be developed. The framework should identify the key stakeholders with an interest and resources for the initiative and the lead agency or agencies should be identified; the role of the International Joint Commission also should be defined. Identification of stakeholders will likely be iterative, with additional stakeholders included as the vision for the products of the initiative develops. The potential reach of the initiative in terms of the number of potential stakeholders is vast, so a stable core management team is recommended to provide continuity and focus over time.

The management framework should be developed with the flexibility to include and build on research already underway by government agencies and universities while also tending to the long-term vision of the IJC Science Advisory Board for a modeling platform.

The form of the initiative should be more clearly defined. For instance, the purpose of the framework may be to establish an environment for model development by a range of actors, including protocols for model comparison, similar to the IPCC approach to global climate model development. Alternatively, the framework may be to establish a forum for binational collaboration to develop a model or group of models to respond to a set of well-defined questions.

Scientific/Technical Collaboration

A conceptual model for the surface-subsurface system is needed to facilitate modeling initiatives and inter-model comparisons. The surface watershed perimeter of the basin does not spatially represent the aquifers contributing to the surface water features of the basin (i.e. the lakes, rivers, wetlands); this spatial complexity needs to be represented in a conceptual model for the surface-subsurface system. In addition, a clear need emerged for harmonized, transboundary subsurface information for the Great Lakes basin. Based on the experience with the Milk River aquifer, undertaking this step will assist in bringing stakeholders together and in defining questions for the modeling initiative. It will also assist in identifying available datasets and key data gaps.

A strategy for data harmonization, data sharing and data access among stakeholders is needed, although the details will depend on the management framework and form of the initiative (discussed above). Similarly, once the model needs are defined, inter-modal comparisons should be planned, including common elements to enable direct comparisons (such as a forcing dataset and a land use dataset to be used).

During the workshop, researchers were informally identifying opportunities to collaborate on studies, shared protocols and other pilot initiatives. The core agencies (USGS, NOAA, NRCan, ECCC, MECP, state governments) should encourage opportunistic pilot studies using existing products while strengthening working relationships among researchers.

7.2 Preliminary plan

This preliminary plan assumes the preferred approach is to develop a modeling framework to facilitate interagency collaboration, stakeholder engagement, data sharing and harmonization, inter-comparison studies and, eventually, to play a role in facilitating stakeholder access to data, model code(s) and other information for regional and local-scale studies. Although specific GW-SW modeling activities can proceed in an *ad hoc* manner, a framework will better serve to fulfill the Science Advisory Board's vision for a comprehensive modeling platform. The preliminary plan includes elements of support, funding, expertise and core scientific activities.

Support

It is necessary to seek IJC endorsement through the Science Advisory Board and the Annex 8 Subcommittee of the Great Lakes Water Quality Agreement for the development of a management framework for an integrated GW-SW modeling initiative (with elements as indicated above). These endorsements would be in principle, initially, to prepare recommendations for outcomes, budget and schedule, and should include seed funding to proceed. With the endorsements in place, an inter-agency steering committee could be established to raise the profile of the integrated GW-SW modeling initiative by consulting with potential stakeholders, funding agencies, and others who can contribute inkind resources. Stakeholders can be engaged to build further support, identify potential funding sources, further define modeling needs, and to refine planned activities to advance the initiative.

Management framework steering committee

An inter-agency steering committee should be assembled to develop the management framework for GW-SW modeling (see 7.1 above) and to report to the IJC through its Science Advisory Board and Annex 8 Subcommittee on planned outcomes, resource requirements and schedule. In parallel with the management framework development, the core agencies should support opportunistic studies that are consistent with the objectives to model basin-scale integrated GW-SW interactions and that build inter-agency relationships and capacity.

Conceptual model

In parallel with refinement of the management framework, the agencies responsible for managing groundwater and surface water in the Great Lakes basin should establish a budget with pooled funding to undertake the development of a transboundary hydrologic conceptual model, including stakeholder engagement and refinement of key questions for basin-scale integrated GW-SW modeling. An inter-agency task force of science experts should guide this work.

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Personal Communications (see also Appendix A and Appendix B)

Scott Bates, Ontario MNRF
Boyan Brodaric, Geological Survey of Canada
Brian Cosgrove, NOAA
Bruce Davison, ECCC
Sandra Eberts, USGS
Daniel Feinstein, USGS
Pradeep Goel, MECP
Norm Grannemann, USGS (retired)
Drew Gronewold, NOAA
Randy Hunt, USGS
Vincent Fortin, ECCC
Valeriy Ivanov, University of Michigan
René Lefebvre, INRS
Scott MacRitchie, MECP
Rich Niswonger, USGS
Al Pietroniro, ECCC
Howard Reeves, USGS
Catherine Riseng, University of Michigan

Jeff Starn, USGS
Ed Sudicky, University of Waterloo and Aquanty Inc.
René Therrein, Université Laval

Appendix A

List of Scientists Participating in the Survey

Name	Affiliation
Scott Bates	Ontario MNRF
Boyan Brodaric	Geological Survey of Canada
Martyn Clark	NCAR
Brian Cosgrove	NOAA
Steven Frey (participated with Ed Sudicky)	Aquanty Inc.
Pradeep Goel	MECP
Drew Gronewold	NOAA
Eloise Kendy	The Nature Conservancy
Randy Hunt	USGS
Vincent Fortin	ECCC
Valeriy Ivanov	University of Michigan
René Lefebvre	INRS
Scott MacRitchie	MECP
Rich Niswonger	USGS
Al Pietroniro	ECCC
Alfonso Riviera	Geological Survey of Canada
Jeff Starn	USGS
Ed Sudicky	University of Waterloo & Aquanty Inc.
René Therrein	Université Laval
Harvey Thorleifson	Minnesota Geological Survey
Eric Wood	Princeton University

Appendix B

Workshop Participants

Name	Affiliation
Richard Berg	Illinois State Geological Survey
Jennefer Boehme	IJC
Mark Burrows	IJC
Philip Chu	NOAA – Great Lakes Forecasting
Serban Danielescu	ECCC
Bruce Davison	ECCC
René Drolet (facilitator)	Rene Drolet Consulting Services
Sandra Eberts	USGS
Mike Fienen	USGS
Katelyn Fitzgerald	National Center for Atmospheric Research
Steven Frey	Aquanty Inc.
Pradeep Goel	MECP
Norm Grannemann	USGS (Retired)
Drew Gronewold	NOAA
Dave Hamilton	The Nature Conservancy
Alan Hamlet	University of Notre Dame
Andrea Hernandez	MIDEQ
Steve Holysh	Toronto and Region Conservation Authority
Randy Hunt	USGS
Valeriy Ivanov (Day 1 only)	University of Michigan
Anthony Kendall (by phone – Day 1 only)	Michigan State University
René Lefebvre	INRS
Paul J. Martin	Matrix Solutions Inc.
Michael Mezzacapo	IJC
Yves Michaud	Geological Survey of Canada
Jim Nicholas	Nicholas-h2o
Rich Niswonger	USGS
Al Pietroniro	ECCC
Elizabeth Priebe	Willet Green Miller Center – MONDM
Howard Reeves	USGS
Alfonso Riviera	Geological Survey of Canada
Hazen Russell	Geological Survey of Canada
Jeff Starn	USGS
Craig Stow	NOAA
Ed Sudicky	University of Waterloo & Aquanty Inc.
Harvey Thorleifson	Minnesota Geological Survey
Mary Trudeau	Envirings Inc.
Jill Van Dyke	MIDEQ
Roland Viger	USGS
Lizhu Wang	IJC
Ram Yerubandi	ECCC

Appendix C

Workshop agenda and materials

1. Workshop agenda

2. Workshop breakout group reporting sheets
    - Day 1:
        - Theme #1: Modeling approach – Identification of key issues
        - Theme #2: Data needs and gaps – Identification of key issues
        - Theme #3: Future applications – Identification of key issues
    - Day 2:
        - Advice for path forward

International Joint Commission

SAB-RCC Groundwater-Surface water modeling for the Great Lakes basin
Great Lakes Environmental Research Laboratory
4840 S. State Road, Ann Arbor, MI 48108
April 4-5, 2018

Meeting objectives:

Convene a group of experts to provide input for consideration by the IJC to:

1. Select and develop a modeling approach to assess the water balance at the basin scale through combined representation of surface and subsurface hydrological processes;
2. Understand the gaps and limitations associated with various options for modeling approach; and,
3. Understand the implications of modeling choice for future work on water quality and ecosystem health.

AGENDA

DAY 1:

9:00 – 9:15	**Opening Remarks**	Norm Granneman, USGS
9:15 – 10:15	**Vision for the Model**	Yves Michaud, NRCan Howard Reeves, USGS René Lefebvre, INRS
10:15 – 10:30	Health Break	
10:30 – 11:15	**Findings from Literature Review**	Mary Trudeau
11:15 – 12:30	**Theme #1 – Modeling Approach**	Drew Gronewold, NOAA
	Presenter	Randy Hunt, USGS
	Commenters	Ed Sudicky, University of Waterloo & Aquanty
	Followed by a facilitated plenary discussion	
12:30 – 1:30	**Networking Lunch**	
1:30 – 2:30	**Theme #2 – Data needs and gaps**	Hazen Russell, NRCan
	Presenter	Roland Viger, USGS
	Commenters	Al Pietroniro, ECCC
	Followed by a facilitated plenary discussion	
2:30 – 2:45	Health Break	
2:45 – 3:45	**Theme #3 – Future applications**	Alan Hamlet, University of Notre Dame
	Presenter	
	Commenters	David Hamilton, TNC Steve Holysh, TRCA
	Followed by a facilitated plenary discussion	
3:45 – 5:00	**Identification of key issues**	Breakout groups
5:00	*End of Day 1*	
6:30	Informal social event (details to be announced)	

DAY 2:

9:00 – 9:15	**Welcome and Agenda for the Day**	René Drolet
9:15 – 9:45	**Summary of Day 1**	Mary Trudeau
9:45 – 10:30	**Theme #1: Modeling Approach**	Plenary session
10:30 – 10:45	Health Break	
10:45 – 11:30	**Theme #2: Data needs and gaps**	Plenary session
11:30 – 12:15	**Theme #3: Future applications**	Plenary session
12:15 - 1:00	**Networking Lunch**	
1:00 – 1:45	**Advice for path forward**	Breakout groups
1:45 – 2:15	**Report to Plenary from breakout groups**	
2:15 – 2:30	**Concluding Remarks**	Sandra Eberts, USGS
2:30	*End of workshop*	

International Joint Commission Workshop
Groundwater-Surface water modeling for the Great Lakes Basin
Ann Arbor, MI – April 4-5, 2018

Breakout session #1: April 4 – 3:45pm-5:00pm
Theme #1: Modeling Approach – Identification of key issues

Table Number: Note Taker:

Question 1: With respect to today's panel discussion on this theme, what are the key outcomes and conclusions for which there is consensus among table members?

Question 2: What are the areas where participants have diverging opinions?

Question 3: What are your top key outstanding issues that should be further discussed during Day 2 of this workshop? (Please list between 1 and 3).

International Joint Commission Workshop
Groundwater-Surface water modeling for the Great Lakes Basin
Ann Arbor, MI – April 4-5, 2018

Breakout session #1: April 4 – 3:45pm-5:00pm
Theme #2: Data needs and gaps – Identification of key issues

Table Number: Note Taker:

Question 1: With respect to today's panel discussion on this theme, what are the key outcomes and conclusions for which there is consensus among table members?

Question 2: What are the areas where participants have diverging opinions?

Question 3: What are your top key outstanding issues that should be further discussed during Day 2 of this workshop? (Please list between 1 and 3).

International Joint Commission Workshop
Groundwater-Surface water modeling for the Great Lakes Basin
Ann Arbor, MI – April 4-5, 2018

Breakout session #1: April 4 – 3:45pm-5:00pm
Theme #3: Future applications – Identification of key issues

Table Number: Note Taker:

Question 1: With respect to today's panel discussion on this theme, what are the key outcomes and conclusions for which there is consensus among table members?

Question 2: What are the areas where participants have diverging opinions?

Question 3: What are your top key outstanding issues that should be further discussed during Day 2 of this workshop? (Please list between 1 and 3).

International Joint Commission Workshop
Groundwater-Surface water modeling for the Great Lakes Basin
Ann Arbor, MI – April 4-5, 2018

Breakout session #2: April 5 – 1:00pm-1:45pm
Advice for Path Forward

Table Number: Note Taker:

Question: Based on the discussion during the whole workshop, identify your Top 3 priorities for next steps and recommended actions. Rank them and for each of them, identify who should be the lead and who else should be involved.

Priority #1

Priority #2

Priority #3

Lack of consensus? If your group has not come to consensus on the top three priorities, please identify the additional priority (priorities) that was (were) considered among the top three by a sub-set of the group and why it (they) should be substituted in for one of those listed above.

____