Final Report

Barrie, Lovers, and Hewitt Creeks – Ecologically Significant Groundwater Recharge Area Assessment and Sensitivity Analysis

Prepared for:

Lake Simcoe Conservation Authority 120 Bayview Parkway Newmarket, Ontario, L3Y4X1



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June 2012



Earth Science Information Systems

June 13, 2012

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RE: Final Report: Barrie, Lovers, and Hewitt Creeks – Ecologically Significant Groundwater Recharge Area Assessment and Sensitivity Analysis

Dear Ms. Howson:

Earthfx is pleased to submit the final report for the Barrie, Lovers, and Hewitt Creeks – Ecologically Significant Groundwater Recharge Area (ESGRAs) Assessment and Sensitivity Analysis. This report summarizes the findings of the previous Technical Memorandums and draft reports. It also provides a description of steps taken by Earthfx to improve on how the model represents the hydrogeologic system within the study area and the surface water features deemed to be ecologically significant.

Another key component of this memorandum is the description of the methodology that Earthfx developed and applied to delineate the source areas for a set of ecologically significant sites. This task served as a test of the capabilities of the revised Tier 2 model for ESGRA assessment.

We appreciate the opportunity to work with LSRCA on this study. Please call if you have any questions regarding this report.

Yours truly, Earthfx Inc.

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1 Introduction

A Tier 2 water budget was completed for the for the South Georgian Bay-West Lake Simcoe (SGB-WLS) study area under the Source Water Protection Program to comply with the 2006 Clean Water Act. The Tier 2 study is documented in a draft report by AquaResource and Golder Associates Ltd (AquaResource and Golder, 2010). The Tier 2 study includes the Barrie, Lovers and Hewitt Creek watersheds which are the subject of the current study (Figure 1). The Tier 2 study used data supplied by a PRMS-based hydrologic model built by Earthfx (2010) to identify the significant groundwater recharge areas (SGRAs) within the portions of the Tier 2 study area falling inside the Lake Simcoe watershed. The SGRAs identified in the study area are shown in Figure 2. While identifying SGRAs is an important task, it is not a certainty that these areas coincide with ecologically significant groundwater recharge areas (ESGRAs). To establish ecological significance, a linkage must be identified between the recharge area and an ecologically significant feature (e.g., a reach of a cold water stream, a Provincially-Significant Wetland (PSW), or an Area of Natural or Scientific Interest (ANSI)).

Earthfx had examined several techniques for identifying ESGRAs and establishing linkages between the recharge zones and ecologically significant discharge areas using groundwater models as part of earlier Tier 1 SWP studies for the Central Lake Ontario Conservation Authority (CLOCA) and the Toronto and Regions Conservation Authority (TRCA). As an example, linkages where defined by using backward particle tracking from areas mapped as potential groundwater discharge areas (identified based on the interpretation of aerial thermography data) and from sites with documented presence of brook trout. Backward tracking was also used to delineate source areas for points along the stream that the model identified as having high rates of groundwater discharge. Based on this experience, Lake Simcoe Region Conservation Authority (LSRCA) retained Earthfx to develop a methodology that allowed for the use of the existing SGB-WLS Tier 2 groundwater flow model to define the groundwater recharge areas that help maintain significant features such as cold water stream reaches and groundwater-fed wetlands within the Barrie, Lovers, and Hewitt Creek watersheds.

2 Study Approach

To establish ecological significance for a recharge area, a linkage must be established between the recharge area and the ecologically significant feature. Establishing a linkage requires:

- identifying the ecologically significant features;
- a conceptual understanding of the local hydrogeology and the factors affecting groundwater/surface water interaction;
- the ability to represent this conceptual understanding with a numerical model;
- the technical ability and tools to trace the movement of groundwater from the feature back to the point where the recharge entered the subsurface (hereinafter referred to as *particle endpoints*);
- a method for evaluating or scoring groups of particle endpoints produced by the model to establish whether they are truly significant; and
- an analysis of the sensitivity of model results to small changes in model parameters, model construction, or model assumptions that could produce large changes in the ESGRA delineation.

LSRCA identified a range of features deemed to be ecologically significant within the Barrie, Lovers, and Hewitt Creek watersheds. These included headwater streams, coldwater fisheries, wetlands,

and brook trout and sculpin capture sites. These are discussed in the following section with respect to how these features were represented in the Tier 2 model.

The physical setting and the development of a three-dimensional conceptual geologic/hydrogeologic model is described in a report by Golder and AquaResource (2009) and summarized in AquaResource and Golder (2010). A description of the conceptual geologic/hydrogeologic model is provided in Section 3.1.4. As part of the current study, Earthfx conducted an assessment of the geology and hydrostratigraphy, as represented in the Tier 2 numerical model, within the Barrie, Lovers, and Hewitt Creek watersheds with an emphasis on the shallow groundwater flow system.

The numerical model developed for the Tier 2 study area is based on the finite-element FEFLOW code (DHI-WASY Software, 2011). The FEFLOW code has the capability to backward-trace groundwater flow paths from points of interest back to the source area for recharge, as well as the ability to use forward-tracking techniques to trace groundwater flow paths from source areas to points of discharge. Application of these tools provided the technical capability to establish linkages between the ecologically sensitive areas and their source of recharge. As part of developing a methodology for delineating ESGRAs, particle tracking with the Tier 2 model was attempted. Limitations in the applicability of the model were identified and are discussed in Section 3. Revisions were made to the model by Earthfx to address these limitations and to add additional surface water features to the model such as headwater stream and wetlands. Model revisions are also discussed in Section 3.

Particle tracking was conducted with the revised model in the Barrie, Lovers and Hewitt Creek watershed. Alternative methodologies were evaluated regarding initial particle placement and sensitivity to variations in particle placement was assessed. Cluster-analysis techniques were developed and tested to assign significance levels to the particle endpoint distributions. In addition, the sensitivity of model results to small changes in model parameters was evaluated. Results are discussed in Sections 4 through 6 of this report.

3 Model Assessment

Earthfx conducted a review of the SGB-WLS Tier 2 groundwater model at the outset of this study. An appreciation of the original purpose and scope of the model development was kept in mind when assessing the suitability of the model for ESGRA analysis.

In the case of the Tier 2 FEFOW model, the model was developed to assess regional groundwater flow patterns as part of a watershed-scale water budget analysis. The analysis focussed on quantifying flow through the groundwater system for use in stress assessment calculations, specifically to estimate water supply (i.e., total water available to the watershed from recharge and lateral groundwater inflow across subwatershed boundaries), water reserve (i.e., water needed to maintain ecological features and, thus, not available for use), and water demand in each subwatershed. The primary objective of the groundwater model was to assess lateral groundwater inflow across subwatershed boundaries. While SGRA delineation was a component of the Tier 2 study, ESGRA analysis and, more specifically, particle tracking was not a component of the Tier 2 study.

3.1 Model Construction

3.1.1 Model Mesh

The FEFLOW code uses the finite-element technique to solve the groundwater flow equation at the nodes (vertices) of a triangular mesh representing the study area. The study area is also subdivided vertically such that uppermost set of nodes, located on the uppermost horizontal "slice" across the study area represents the top of Layer 1 while the set of nodes on the next slice represents the bottom of the Layer 1 and top of Layer 2. Hydraulic properties are assigned to each triangular prism formed by the nodes.

In FEFLOW, the construction of the finite-element mesh is automated, with the option to refine the mesh around specific areas of interest, such as pumping wells or rivers, with the objective of better representing the geometry of physical features and to follow naturally complex boundaries such as the Niagara Escarpment. The Tier 2 model mesh was refined in areas where it was felt to be important to have an enhanced definition of groundwater flow and the potentiometric surface. This included areas beneath and surrounding the major rivers and streams represented in the model and near large groundwater takings (Figure 3).

An obvious disadvantage of refining the mesh around a select number of features is that (1) the grid is not refined where features such as streams or wetlands were assumed to be of lower significance (with respect to the subwatershed water balance, but not necessarily from an ecological perspective) and (2) the grid needs to be re-designed whenever a new feature is added.

3.1.2 Lakes, Streams, and Wetlands

Explicitly representing the ecologically significant surface water features, such as lakes, wetlands, and streams, is a key requirement if the model is to be used to establish linkages to the ecologically significant recharge areas. For example, if wetlands in low-lying areas and riparian zones serve as broad zones of diffuse groundwater discharge; these features should be represented numerically as groundwater discharge zones. If groundwater discharge to a large number of headwater streams contributes to flow in the main reaches, then both the headwater streams and main reaches should be represented in the numerical model.

As noted earlier, LSRCA provided Earthfx with digital files identifying sensitive features within the study area. These features included coldwater fisheries, known brook trout and sculpin capture sites, and wetland areas. These locations, along with wetland mapping provided by the MNR, were overlain on the model grid to verify that these features were represented in the FEFLOW model. A number of serious limitations were identified in this exercise as discussed below.

<u>Lakes:</u> Only four interior lakes within the Tier 2 model area exceeded a threshold of 0.5 km² and were simulated in the model. No significant lakes are located within the watersheds for the Barrie, Hewitt, and Lovers Creeks, so this was not a significant issue for this study. Kempenfelt Bay is represented as a constant head boundary across several model layers.

<u>Streams:</u> Only the streams reaches shown in Map 4-3 of the Tier 2 Report (AquaResource and Golder, 2010) are simulated in the Tier 2 model. A comparison between the actual and simulated stream network is shown in Figure 4 and Figure 5. The reaches represented in the model are mostly the higher-order reaches (Strahler Class 4 and above) and represent only the main channels of Barrie, Lovers and Hewitt Creeks. It is recognized that some of the headwater streams and minor tributaries may be intermittent (where the stream base is close to or above the water table during much of the year) and therefore may not contribute significantly to the subwatershed water budget

on an annual average basis. However, representing only the higher-order reaches of a stream network forces the groundwater flow paths to converge on the lower reaches, whereas, in the real system, groundwater may discharge preferentially to the more numerous lower-order tributaries and headwater springs. Tracking back from the high-order streams may lead to errors in identifying the source areas while tracking back from the low order streams is impossible because they are not represented in the model. The FEFLOW mesh was refined to represent the corridors around the larger streams, although these were mapped using a series of coarse line segments that considerably simplified the actual stream configuration (Figure 4 and Figure 5). Stream nodes were separated by about 50 m and the width of the refined stream corridor was approximately 200 m.

Streams were represented numerically as specified (constant) head boundaries. Stream stage assigned to the constant head nodes was derived from topographic mapping and was assumed to remain constant in the steady-state simulations. This representation is appropriate for the large streams. Representation of smaller streams as constant-head boundaries, however, can often lead to errors. For example, if the choice of other model parameters (e.g., aquifer hydraulic conductivity and/or recharge rates) would cause the simulated head to be below the stream base in an area where the stream is known to be a groundwater discharge zone, assigning a constant head will artificially raise the water levels and cause the "stream" to supply an unconstrained amount of recharge to the aquifer. This appears to be the case for several of the headwater streams in Lovers and Hewitt Creek as well as for other streams outside the study area. These unconstrained boundaries supply a significant amount of water to the watershed. They also caused particle tracks from the main stem of Lovers Creek to trace back to the headwaters in our preliminary simulations. This problem and remedies are discussed further in Section 3.3.

The hydraulic conductivity of Layer 1 was adjusted to represent the streambed material. Extremely low values of hydraulic conductivity were assigned to the elements representing some stream beds, for example, those in the Barrie Creeks watershed. At the same time, a reasonable rate of recharge was applied to the same elements. This combination of model parameters used in applying the stream boundary conditions caused anomalously high heads in the stream corridors in the Barrie Creeks watershed. Figure 6 shows a screen capture from the FEFLOW model showing heads in Layer 1 in the Barrie Creeks watershed (near Kidds, Bunker, and Dyment Creeks). Heads at the streams are up to 120 m above local land surface topography and in some cases up to 80 m above local topography in the underlying layers.

<u>Wetlands:</u> Minesing Swamp is the only wetland represented in the Tier 2 model. There are between 160 (MNR mapping) and 206 (ELC mapping) separate wetland areas in the Barrie, Hewitt, and Lovers Creeks watersheds that are not represented in the FEFLOW model as wetlands. Locations are shown in Figure 7. The wetlands and riparian features illustrated in Figure 7 are likely areas of groundwater discharge; however, they were not built into the FEFLOW model. Consequently, these features were likely misrepresented as areas of groundwater recharge similar to the surrounding area, which makes it difficult, if not impossible, to trace the source of recharge (ESGRAs) to these features. Fortunately, many of the riparian wetlands have stream reaches running through them so that at least a proportion of these wetland areas act as a groundwater discharge zone in the model.

<u>LSRCA Sensitive Feature Mapping</u>: Of the 16 temperature sites classified as "cold water" for assessment, 5 are on tributaries represented in the model (Figure 8). Of the 22 brook trout capture sites that are identified, 15 are coincident on simulated stream reaches (Figure 9). Of the 14 sculpin capture sites, 13 are on represented reaches. The rest are on tributaries not represented in the Tier 2 model (Figure 9).

3.1.3 Recharge

Groundwater recharge refers to the amount of water that infiltrates the soil surface, percolates downward through the unsaturated zone, and ultimately reaches the water table. The rate of groundwater recharge is dependent on a number of factors, including precipitation, land use and vegetation, surficial soil type (geology), physiography, and ground surface topography.

Recharge values for the FEFLOW model were obtained from two separate surface water models developed for the SGB-WLS area. One recharge model was developed for the Nottawasaga Valley and Severn Sound watersheds (NVCA, 2010) using the U.S. Environmental Protection Agency Hydrologic Simulation Program - FORTRAN (HSPF) code (USEPA, 1997). A second recharge model was developed by Earthfx (2010) for the Lake Simcoe watersheds using a modified version of the U.S. Geological Survey Precipitation-Runoff Modeling System (PRMS) code (Leavesley et al., 1983). Annual average recharge rates, as determined by the models, are shown in Figure 10.

The PRMS model was developed as part of a regional-scale assessment of the water balance in the Lake Simcoe Basin using available data on climate, soil properties, land use, and topography. The model was intended to provide a better understanding of watershed behaviour on a seasonal and annual basis and to provide a greater understanding of the interaction of streams, wetlands, and the groundwater systems. Model results included estimates of water budget components (i.e., precipitation, interception, runoff, infiltration, evapotranspiration (ET), groundwater recharge, and baseflow) on a daily, monthly, seasonal, and average annual basis. The model was run for Water Years 1975 to 2002 and calibrated to match observed flows and estimated baseflow values at multiple gauges within the study area. Estimated annual groundwater recharge rates averaged over the 27 year period were used in the Tier 2 model.

Within the PRMS model, wetlands and inland water bodies in the Lake Simcoe basin were treated as being 99% impervious. This was done assuming that groundwater is discharging to the wetland over most of the year and, thus, recharge does not occur. Wetlands in Lake Simcoe basin are mostly located in riparian zones surrounded by upland till plains; therefore stage in these wetlands is likely lower than in the underlying aquifer and thus recharge is not occurring. It is also assumed that these land types have standing water for most of the year and that changes in wetland storage are negligible. Increased ET was accounted for by increasing the depression storage capacity and allowing evaporation from depression storage to represent evaporative losses from standing water and wetland vegetation. Depression storage for all wetlands was set to a depth of 2.54 cm.

In summary, the PRMS model was adjusted to account for the lack of groundwater recharge in wetland areas. This assumption had to be made as the PRMS model was not coupled to a groundwater model and thus could not account for groundwater feedback mechanisms. ET and evaporative losses were represented by taking water out of a representative depression storage reservoir. Groundwater discharge to the wetland was not simulated directly in the PRMS model as it was assumed that this would be done explicitly in the groundwater model. This expected discharge to the wetlands and riparian areas, however, was not represented in the Tier 2 groundwater model.

3.1.4 Hydrostratigraphic Model Layers

To facilitate the review of the geological model, the FEFLOW surfaces were imported to VIEWLOG. The conversion from FEFLOW to VIEWLOG allowed Earthfx to visually review the geological surfaces in both plan view (either "top of" or "thickness of") and in cross section with local borehole data.

The Tier 2 model was developed based on several conceptual models from earlier studies, which were adapted to represent conditions in different parts of the Tier 2 study area. The representation of the lithographic units within the geological model differs from conventional geological models, which relate model layers to stratigraphic units (e.g., the Newmarket Till, top of Bedrock). The Tier 2 model layers are presented on Figure 11.

As discussed, the construction of the Tier 2 geological-hydrogeological model does not follow the approach of mapping geological units (by name) based on the lithological descriptions and stratigraphic location/elevation. For example, a regionally extensive aquifer and/or aquitard layer would be represented in the model as two or more hydrostratigraphic layers. Similarly, lithostratigraphic units that have similar elevations but are geographically separate were often combined into a single model layer (Figure 12). Layers 1 through Layer 8 represent the till upland areas in the Barrie area. The till uplands are generally capped by the upper Newmarket Till (Layer 3 and/or Layer 5) but in many places this till is overlain by coarse-grained glaciofluvial deposits (Layer 2 and Layer 4). Layer 7 (SC4) may represent the 'lower Newmarket Till' or an equivalent aquitard. In the deep system, Layer 10 (A2) appears to represent the Thorncliffe Formation (or its equivalent) and the Scarborough Formation aquifers are modelled by layers 12 (A3) and 14 (A4). There is no single surface for the top of bedrock across the Tier 2 area. In the Barrie area, the top of bedrock is represented by top of Layer 16 (Georgian Bay Formation), which clearly displays some incised bedrock valleys.

Sedimentary deposits within tunnel channel complexes beneath the City of Barrie and Kempenfelt Bay are not explicitly represented by model hydrostratigraphic layers. Regardless, it seems that the model does represent significant geological/hydrogeological features (e.g., tunnel channels), not in terms of stratigraphy, but by varying the hydraulic properties laterally within model layers. We did not review model property values for the lower layers. The model has been subject to external peer review and we assume that the values used were analyzed in this review. Model calibration is discussed below.

3.2 Tier 2 Model Calibration

Calibration of the Tier 2 model and results of model simulations, including simulated heads, residuals, and calibration statistics, are discussed in the Tier 2 Report. Model calibration is a process that attempts to minimize the average residual over the entire model area. Local discrepancies between simulated and observed heads may exist. In general, the model tended to underpredict heads (by over 20 m) in the Lovers and Hewitt Creek subwatersheds. Heads were too high (by over 20 m) in the Barrie Creeks subwatershed. In discussing the calibration to estimated baseflow, AquaResource and Golder (2010) note that:

"In general, the fit to observed flows along large stream reaches is good; however, the fit is not as good for smaller reaches. This is to be expected, as the numerical model has not been developed to represent local hydrogeologic conditions, but rather, to represent regional conditions."

However, calibration to stream flows does not mean that the model accurately represents the stream flow conditions. As discussed in Section 3.1.2, incorrectly representing stream reaches using unconstrained constant head nodes makes it difficult to impossible to trace the source of recharge to the area using the provided model design.

3.3 Need for the Model Update and Correction

Following the model review and after unsuccessful attempts to conduct forward and backward particle tracking with the model, a number of issues were identified as significant limitations to the application of the model for ESGRA assessment.

3.3.1 Stream Boundary Condition

The most significant problem identified in the Tier 2 model is the incorrect configuration of specified head boundary conditions in the upstream portions of many of the tributaries. The model is "injecting" significant quantities of water at these unconstrained fixed-head nodes. The position of these nodes is shown in Figure 14 (orange-red dots). The problem, shown schematically in Figure 15, is that the stream headwater nodes are defined as constant head nodes at an elevation above the predicted elevation of the water table. To maintain the water level at the defined stream node the model "injects" water a rate necessary to sustain the fixed water-surface elevation at the node.

The impact of this error is significant to both the water budget and the simulated flow patterns. The total injection node flow is equal to about 67% of the surface recharge applied to the Lovers Creek watershed (see Table 1). The injection nodes represent unconstrained inflows added to the water budget beyond that determined by the recharge model.

The impact of these nodes on the flow system patterns is also significant as the injection node inflows are, in many cases, locally greater than the recharge applied in the SGRAs. Preliminary reverse particle-tracking from many of the defined ecological features led back to the headwater injection nodes instead of the SGRAs.

This problem occurs throughout the Tier 2 model, including the Hewitt Creek watershed. The legend used in Map 4-10 of the Tier 2 report somewhat obfuscates this issue by lumping all river leakage nodes into one colour category (<0), while using multiple color categories for groundwater discharge. The transient analysis of drought condition response would also be affected by the unconstrained constant-head nodes. These unconstrained boundary conditions would supply additional water to maintain the water table elevation even when recharge is reduced.

3.3.2 Water table above Land Surface

Together with these excessive inflows; poor model configuration and calibration in the vicinity of the main stream reaches results in extensive areas where the predicted water level is above ground surface in the stream valleys. Significant portions of the Lovers Creek valley are inundated (Figure 16 and Figure 17) in the model. While this issue may only represent an error confined to a localized area within the shallow flow system (and therefore would not significantly affect the regional water budget), the limitations in the particle tracking module in FEFLOW make this a significant problem for ESGRA analysis.

Limitations of the FEFLOW particle tracking module when the water table is above and surface apply to both forward and reverse particle tracking. When forward tracking, the particle-tracing algorithm incorrectly identifies points where the heads exceed land surface as the exit points for the particles. Shallow forward particle tracks stop at the point where the water level exceeds ground surface (red dots in Figure 18b) and therefore the particles never reach the stream or ecological feature of interest.

Similarly, when backward tracking from the modelled stream channel only a limited number of paths are delineated. All of the shallow particles released in areas where the water table is above ground surface follow the direction of flux upwards, and therefore prevent backwards tracking to significant features. Only those particles that travel deeper paths through the aquifer (underneath the high water table zone) move to their point of recharge (see Figure 18c).

These two issues, (i.e., the poor calibration within the stream valley and the technical limitations of FEFLOW particle tracking when heads are above ground surface) make it impossible to delineate ESGRAs with any certainty using the model as currently configured. This problem is not restricted to Lovers Creek and exists in many other watersheds in the Tier 2 model.

3.3.3 Water Level Mounds near Warm Water Streams

A third problem exists in the vicinity of the streams in the Barrie Creeks watershed. The PRMS model estimated a recharge rate of about 225 mm/yr for the alluvial deposits in the vicinity of the streams. As noted earlier, the hydraulic conductivity for the streambed elements representing alluvial deposits in warm-water creeks was set to 1×10^{-9} m/s, a very low value. This discrepancy between the surficial geology, estimated recharge, and Layer 1 hydraulic conductivity causes a large M-shaped groundwater mound to develop in the alluvium around the stream. Predicted water levels in the vicinity of the streams greatly exceed land surface, appearing as "spikes" shown in Figure 16, the contoured highs in Figure 6, and schematically in Figure 19.

This condition occurs most notably in the vicinity of the Barrie Creeks but also occurs at other warmwater creeks in the Tier 2 model. Particles cannot be reliably traced back to ESGRAs under these conditions.

3.4 Model Update and Refinement for ESGRA Analysis

After model review, the decision was made by LSRCA to update the model within the study area to address some of the limitations identified. The changes to the model were limited to modifications of the boundary conditions, stream and wetland representation, and refinement of the hydraulic conductivity of the upper layers to better represent the shallow flow system and water table. Structural changes to the model mesh and conceptual model were considered beyond the scope of this project. The following changes were implemented:

3.4.1 Removal of Injection Nodes

The first change to the model was the removal of the unconstrained first-type boundary condition nodes that were "injecting" water into the headwaters. Removal of these unconstrained boundaries caused changes in the position of the water table. Accordingly, the hydraulic conductivity of the upper model layers needed to be adjusted downward to increase water levels in areas where the streams were likely to be gaining. The removal of the injection nodes also prompted an overall assessment of the headwater stream representation. These two items are discussed further below.

3.4.2 Refinement of Stream Representation

The limited representation of the stream network in the existing FEFLOW model (Figure 4) was addressed by reviewing the mapped streams and adding additional stream details into the model.

Cauchy or third-type boundary conditions are the preferred mechanism for representing headdependent discharge that occurs along stream reaches. Cauchy boundary conditions cannot be applied to nodes or lines in FEFLOW; they can only be applied on an elemental basis. This, coupled with the relatively coarse mesh used in the model, made Cauchy boundaries a poor choice to represent the smaller headwater streams without significantly refining the model mesh.

An alternative approach was identified using constrained first type constant head nodes. While the original model was constructed using *unconstrained* first type nodes, it was the lack of a constraint on the nodes that allowed the erroneous injection of water into the model. By adding a constraint (limiting the constant head to allow only outflow), stream discharge could be simulated without the artificial injection of water in locations where the water table was below the stream bed elevation. This approach effectively replicated the Cauchy boundary approach but on a nodal basis.

Using this approach, several stream segments were added to the model as shown in Figure 20. These helped to lower the water table in areas where the original water table was well above land surface. Existing unconstrained first-type model boundary nodes were also converted to constrained first-type nodes both inside and outside of the study area. While a number of additional stream reaches were added, the coarse nature of the mesh prevented us from adding all stream reaches to the model. The coarse mesh also prevented us from closely matching the stream channel configuration. To properly represent these streams, a redesign of the model mesh would be required.

In summary, this refinement improved the model in the following ways:

- 1. additional stream segments were represented in the model;
- 2. constant head nodes were constrained to eliminate the artificial injection of water; and
- 3. the addition of streams helped to lowered the water table to ground surface in the stream valleys, thereby improving particle tracking results.

3.4.3 Addition of Wetlands

While Cauchy boundary conditions cannot be applied at nodes in FEFLOW, they could be used to represent the areal discharge of groundwater that occurs under wetlands elements. While no wetlands were represented in the original model, triangular model elements corresponding to the larger wetlands in the study area were added as shown in Figure 21. The addition of wetlands helped to further lower the water table to ground surface in the stream valleys.

3.4.4 Refinement of Upper Layer Hydraulic Conductivity

Once the changes to the boundary conditions were made, the upper layer hydraulic conductivity was locally refined. It should be noted that this refinement was limited to the shallow zones within the study area watersheds and not for the whole model or for deeper layers. The refinements included:

• adjustment of the extremely low streambed hydraulic conductivity in Layer 1 that caused the water table peaks in the vicinity of the Barrie Creeks (Figure 22);

- slightly reducing the hydraulic conductivity of Layer 2 in a broad area within Lovers Creek watershed and increasing the hydraulic conductivity in a circular zone east of Hewitt Creek (Figure 23);
- reducing hydraulic conductivity in Layers 3 and 4 (Figure 24 and Figure 25) in a large "window" that had apparently been created under Lovers Creek (little evidence for the window could be found in the well log data); and
- adjustments to the vertical hydraulic conductivity distributions (Figure 26 through Figure 29).

3.4.5 Model Refinement Results

Results of model refinement, as indicated by the updated simulated water table, are show in Figure 30. This figure can be compared against Figure 31 which shows the simulated heads in the original Tier 2 model. The water table no longer exhibits the mounds and peaks and less of the model area is inundated (water table above ground surface). In general, the predicted water table provides both a reasonable representation of the local topographic controls and more regional flow towards the Barrie well fields.

Unfortunately there are only a few shallow wells in the MOE water well information system (WWIS) that provide an indication of the water table position (at the time of drilling), so the presentation of a statistical analysis of the calibration is not possible.

3.5 Conclusions

The model update has addressed the issues identified in the initial model review phase of the ESGRA study. The following issues have been addressed:

- stream injection nodes have been removed;
- additional streams have been represented in the model based on the existing finite-element model mesh using an improved constrained first-type nodal boundary condition;
- wetlands are represented in model with element-based Cauchy boundary conditions using the existing model mesh; and
- upper layer streambed properties and shallow-layer hydraulic conductivity values have been refined and improved.

These changes improved the model representation of the key surface water features needed to complete the ESGRA assessment.

4 ESGRA Delineation Methodology

The objective of this project was to develop a consistent, objective, and technically sound methodology for the identification and delineation of ESGRAs that can be used for this and future studies in the other Tier 2 subwatersheds.

4.1 Particle Tracking Techniques and Issues

Particle tracking is an accepted methodology for visualizing and understanding groundwater flow paths (Figure 32). It is particularly useful in areas with complex, three-dimensional flow fields. To conduct a particle-tracking analysis, the groundwater model is first used to determine groundwater heads and fluxes at all nodes. A velocity field is then derived from the nodal fluxes. Virtual particles are then traced through the flow field and the point of entry into an element, transit time, and exit point are recorded. Pathlines can be displayed by connecting the points along the flow path. Particle endpoints (i.e., the location at which the flow path intersect land surface) can also be displayed or recorded for further analysis.

Particles can be tracked either in the direction of flow or in the reverse direction. For forward tracking in the direction of flow, particles are usually introduced in a uniform distribution across the model area. The particles can be traced from the point of entry to the point of discharge or to where they exit model boundaries. While forward tracking can help define and visualize the regional flow system, it may be necessary to release an extremely large number of particles to trace those that discharge at ecologically significant locations.

With backward or reverse tracking, particles are introduced in a dense distribution at the point of known groundwater discharge or around ecologically significant features. The virtual particles are then tracked backward using the same velocity field, from the point of discharge to the point of recharge (or to a model inflow boundary). A benefit of reverse tracking is that attention can be focussed on specific known ecological features.

Ideally, the two methods should result in identical results. Practical limits to the number of particles that can be applied uniformly across the model area and limits in the number of particles that can be packed into a discharge area may cause some variations in model results, especially in complex flow fields. For example, if groundwater is moving through widely-spaced "windows" in a regional aquitard, it may be difficult to detect all the windows if only a limited number of particles are released.

One inherent advantage of the backward tracking is that the particle endpoints often converge on specific areas. The density of particle endpoints can be used as an indicator of the significance of the recharge area. The number and initial placement of particles may, however, affect the accuracy of the backward-tracking results: For example, placing particles uniformly across a wetland may yield different results than concentrating the particles along the edges of the wetland where much of the discharge likely occurs.

Other limitations can exist in the particle tracking code implemented within a particular modelling code. As outlined in Section 3.3.2, when the predicted water table is above the top of Layer 1 (land surface) in the FEFLOW model, particle tracking stops when the particle moves above land surface. In other models such as MODFLOW or MODPATH, particles are followed through the inundated zone to the exit point.

In summary, reverse particle tracking from the known ecological features is considered the most useful and direct means of identifying the recharge location. Forward tracking was used in this study to confirm the reverse tracking results and as well as to provide insight into the regional flow field.

4.2 Particle Release Location and Density/Distribution

In addition to the selection of a particle-tracking technique, the number and distribution of particles

released needs to be standardized if the consistent results are to be determined across multiple watersheds, ecological features, and particle tracking scenarios.

FEFLOW can release particles at model nodes, at specific points, and along a tree-dimensional line. Particles released along a line feature or within a specified radius around a node are limited to 1000 individual seeds in the FEFLOW code. This effectively limits the number of path lines that can be easily generated around a specific feature. Particles released around a node can also be placed in a flux-weighted manner, such that a larger number of particles are placed along the arc in the direction of greatest flux. A three-dimensional grid of points theoretically offers the possibility of an unlimited number of particles, however the grids must be created in a third party GIS package (such as ArcGIS or VIEWLOG) and then loaded into FEFLOW as an ArcGIS shape file. In reality, there is an upper limit to the number of particles released based upon the computational resources available to the user.

When backward tracking from stream nodes (as shown in Figure 20), particles were released in a fixed radius around each node. As the stream nodes are nominally spaced 50 m apart, particles were released in a fixed radius of 50 m around the stream nodes to capture the stream centre line and riparian buffer. One hundred particles were released around each node (Figure 33).

Particles were also tracked back from wetland features based on the ELC mapping shown in Figure 7. Because wetlands are represented as elements within the refined model, a grid of evenly spaced particles, 20 m on centre, was released over these features (Figure 34).

Particle release points for coldwater reaches (Figure 8) and brook trout and sculpin capture sites (Figure 9) were established by creating a grid of evenly spaced particles, 5 m on centre, within a 200 m (lateral) by 400 m (longitudinal) buffer area (Figure 35). This method of particle release was chosen to capture riparian zones around these significant reaches.

As an additional analysis, forward tracking of particles from SGRAs and ESGRAs was undertaken by creating a grid of evenly spaced particles, 10 m on centre within these areas. This was done to investigate pathlines that exit the study catchments and to see if recharge in these areas eventually discharges to the ecologically significant areas of concern. Results and sensitivity to the methods selected are discussed below.

4.3 ESGRA Delineation and End Point Cluster Analysis

While reverse particle tracking (with a sufficient number of particles) can link ecological features to a recharge area, defining that recharge area as "significant" implies that it contributes a substantial portion of the total flow volume. Identifying clusters of reverse particle endpoints can be used as a reasonable indicator of flux contribution to a discharge point. A critical component of the study was to develop a method that would allow for a defensible, unbiased, and repeatable scientific method to delineate ESGRAs across different watersheds.

Based on discussions with LSRCA, previous work, and testing done in this study, the preferred method to delineate ESGRAs was determined to be an unbiased endpoint clustering analysis technique. Variants of the proposed methodology were tested as to whether they met the objective of delineating ESGRAs. Various methods and samples were discussed with the Project Team at technical meetings. The details and justification for the bivariate kernel density cluster analysis methodology for delineating ESGRAs, along with a step-by-step description of the process, are presented in Appendix A.

The proposed methodology requires specifying the number of particles released and the parameters of the bivariate kernel density estimator (h, ϵ). Table 2 presents the percent of the total number of endpoints (compared to the number of particles released) considered as part of an ESGRA for various values of the bivariate kernel density estimator (h, ϵ). Table 3 presents the corresponding percent of the total study area delineated as ESGRAs for various values of the bivariate kernel density estimator (h, ϵ). Following testing and discussions with the Project Team, the kernel density smoothing parameter h was set to 25 m, equal to the chosen grid cell spacing for the kernel analysis. A delineation threshold $\epsilon = 100$ was chosen because it proved to consistently identify clusters while meeting the following criteria:

- rejection of endpoints that clearly did not belong to any cluster;
- delineation of clusters with a relatively high density of particle endpoints; while
- avoiding spreading into areas where endpoints did not exist.

In summary, the cluster analysis can be used to convert the endpoint distribution into a uniform gridded parameter that can be contoured, visualized, evaluated for significance, and compared across watersheds and features.

5 ESGRA Delineation Results

As noted, ESGRAs are defined as the areas of land that contribute significantly to the groundwater discharge at points designated as sensitive surface water features (e.g., coldwater stream reaches or wetlands). With the application of the methodology discussed in Section 4, Earthfx has identified the linkage between the ecologically significant surface water features and the recharge areas. Application of the bivariate kernel density estimation technique provided a quantitative method for evaluating cluster endpoint density and delineating the extent of the ESGRAs.

5.1 Backward Tracking and Cluster Analysis

Six representative simulations are presented that delineate ESGRAs of streams (Figure 36), wetlands (Figure 37), brook trout and sculpin capture sites (Figure 38), coldwater reaches (Figure 39), wetlands and coldwater reaches combined (Figure 40), and all features combined (Figure 41). ESGRAs delineated by particle endpoint cluster analysis are compared against the SGRAs mapped previously in the Tier 2 study. A sample of backward-tracked endpoints is supplied in Figure 42, which demonstrates the ability of the cluster analysis to correctly outline dense regions. Endpoints were rejected based on low relative densities. Endpoints having short travel times (less than 1 day) were also rejected.

In both Hewitt and Lovers Creeks, ESGRAs are dispersed around the catchments roughly to the start of the headwater tributaries; whereas in the Barrie Creeks area, recharge is restricted to the stream channels. Forward particle tracking showed a large portion of the recharge within the catchment contributes to the City of Barrie municipal wells rather than to streams (Figure 43). Similarly, there are few contributing areas to wetlands in the mainly urban Barrie Creeks watershed compared with the more rural Hewitt and Lovers watersheds.

The ESGRA results indicate that there is some correlation between SGRA and ESGRA zones, particularly in the west-central portion of Lovers Creek. ESGRA's and SGRAs coincide in the vicinity of Innisbrook Golf Club and McKay Road east of Highway 400. A gravel pit south of McKay Road in the area suggests that coarse grained (high recharge) materials are present in this area. By comparing Figure 36 and Figure 37, however, it is apparent that large discrepancies exist between

the ESGRAs mapped from particle clusters and the SGRAs mapped in previous efforts (Earthfx, 2010). SGRAs may not be coincident with the ESGRAs mapped from particle clusters for the following reasons:

- 1. High recharge rate predicted by surface water models alone cannot indicate ecological significance because of the complexity of the groundwater flow paths; and
- 2. The FEFLOW model used here was not designed for analysing near-surface hydrological process and flow pathways.

ESGRAs delineated by cluster analysis of backward tracking from brook trout and sculpin capture sites are presented in Figure 38. Much of the ESGRAs delineated from these features in the Lovers Creek subwatershed coincided with the mapped SGRAs, although they represent a very small portion of the areas. ESGRAs in the Hewitt Creek watershed showed no correlation with SGRAs and no clusters were identified in the Barrie Creeks watershed. Cluster analysis from these sites was sensitive to whether the mapped capture locations coincided with stream reaches that were explicitly defined in the FEFLOW model. Figure 9 illustrates the selected locations relative to the modeled streams, showing that the majority (19 of 26) of capture sites were located on modelled stream reaches. Comparing Figure 38 with Figure 36 indicated that ESGRAs delineated from brook trout and sculpin capture sites are coincident with the ESGRAs delineated from the stream network.

Figure 39 shows that very few clusters were identified from backward tracking analysis originating from coldwater reaches. Backward tracking from these identified coldwater reaches (where brook trout and sculpin spawning can be assumed to occur) provides little aid in identifying ESGRAs. A larger number of clusters were expected because the backward-tracked particles originated from areas of known groundwater discharge to streams. This again suggests limitations in the ability to simulate near-surface groundwater movement, despite the recalibration efforts. This is due mostly to the coarse discretization away from the stream networks and wells.

Combined ESGRA mapping is provided in Figure 41, which shows ESGRA mapping from all ecological features (streams, riparian zones, wetlands, fish capture sites, and areas of suspected groundwater discharge (cold water reaches)).

5.2 Forward Tracking and Travel Time Analysis

Figure 43 illustrates the generated forward particle tracks from a grid of particles 20 m on centre covering the entire study area. Some forward particle tracks are seen to cross the topographical watershed divide to the west and south. The forward tracking results suggest that the study area watersheds may be a significant source of recharge to other catchments through cross-boundary flow. This should be considered when delineating ESRGA in adjacent catchments, as it may be necessary to expand the study area if cross watershed flows are significant (e.g., the Innisfil Creek catchment).

To verify that the backward tracking method has correctly identified the areas supplying the sensitive ecological features, a forward tracking exercise was also undertaken. Particles were released on a 10 m grid over the ESGRAs for all features (Figure 41) and forward tracked to a final destination (Figure 44). It can be observed that the majority of the particle tracks end either in or adjacent to the stream and wetland features. Particles were also forward-tracked from SGRAs (Figure 45). In this case, many particles cluster around stream channels, but other particles reach the shores of Kempenfelt Bay and the Barrie municipal wells. Because of the cross-watershed boundary flows, some particles released from the SGRAs exit the study area and may help support ecological features in other catchments.

6 <u>Sensitivity and Scenario Analysis</u>

The accuracy of the delineation of ecologically significant recharge areas depends primarily on the accuracy of the FEFLOW model. It has been acknowledged that the original Tier 2 model was not intended for the use to assess ESGRAs; however, it is noted that a model that can reasonably replicate the observed potentials and flow patterns should be able to provide reasonable assessments of the local flow conditions.

While the Tier 2 model has been calibrated to determine reasonable input parameter values (e.g., hydraulic conductivity and recharge rates), particle tracking results may still be sensitive to small changes in these values. The sensitivity of ESGRA delineation to minor changes in these model parameters is presented in the following sections:

6.1 Sensitivity to Number and Placement of Particles Released

Depending on the local hydrogeology, particles may have very complex, three-dimensional flow paths where they travel through multiple aquifers and aquitards. In some settings, particles discharging in a particular wetland or stream may originate from widely dispersed source areas or from multiple locations within a large recharge zone. In these cases, limiting the number of particles used to delineate ESGRAs could lead to errors in identifying the full extent of these areas. The simplest way to test sensitivity to the number of particles is to run the baseline with a reasonable number of particles and then increase the number of particles by a factor and then compare results.

Early on in the study, analyses were completed with varying numbers of released particles to determine the best strategy. Ultimately, the choice of particle release density came down to maximizing the number of particles released while not exceeding the computational abilities of FEFLOW and the computer running the model. Simulations with particle numbers exceeding 100,000 were not manageable.

Various particle tracking start-point densities were investigated. Particle densities surrounding each node and the particle release radii are user-defined and thus were varied to investigate effects on model results. Figure 46 presents results using 100 particles released at all river nodes with a radius of 25 m. This can be compared with Figure 36 showing results using a radius of 50 m. Model results appear quite sensitive to node release radius and show a distinct change in delineated ESGRAs. Total ESGRA delineation for the 50 m radius trial was 35% greater than for the 25 m trial. Testing with a larger radius was not done as this would place particles outside the riparian buffer. Release density showed no distinguishable differences between release densities of 50 particles per node (Figure 47) and 100 particles per node (Figure 48).

A second method of particle release was undertaken from a set of uniformly spaced 3D points to overcome the limitations in the particle release options around selected nodes and the variations in nodal density inherent in the finite-element mesh designed for the Tier 2 model. The particle tracking point grid density was varied from one point per 100 m cell to one point per 5 m cell for identified sensitive features. Generally, increasing particle density was found to produce more concentrated clusters. Reducing the grid spacing to less than 20 m, however, was found to offer little additional cluster resolution.

The particle densities utilized in the latter tests exceeded the memory (6 GB) of the particular computer used. Testing was able to be completed by combining the results of several batch runs.

Final backward tracking grid densities were set to a spacing of 5 m to 10 m to yield an appropriate cluster density while allowing the analysis to be completed in a manageable number of batches.

In summary, the following release densities and distributions were deemed sufficient for the particle tracking exercise:

- backward tracking from streams: 50 m radius around stream channel centreline nodes with 100 particles released per node;
- for reaches in streams specifically identified as ecologically significant, such as brook trout and sculpin capture sites and coldwater reaches, at 400 m (long/tudinally) by a 100 m buffer was delineated around every feature and a release point density was increased to a 5 m spacing;
- backward tracking from wetlands: a 20 m spacing was released from within all ELC wetlands polygons; and,
- forward tracking was found to be sufficient using a 10 m particle spacing originating from all points within the ESGRAs and SGRAs.

6.2 Sensitivity to Flux-Weighted Number of Points Released

The FEFLOW code provides the option to flux-weight the distribution of seeds released around a node. This spaces the points around the node such that the approximate relative flux represented by each particle released is equal. It should be noted that this only balances the flux at each node individually, and not across the model domain. Even with the flux-weighting option enabled, the magnitude of the flux represented by each pathline is relative between nodes.

The sensitivity of delineated ESGRA boundaries to the use of flux-weighting was investigated. At the seed densities employed in the study (50-100 seeds per node), no appreciable change in delineated ESGRA boundaries were observed with flux-weighting enabled. This can be seen by comparing Figure 36, Figure 47, Figure 48, and Figure 49. In addition, this feature is computationally intensive and is not recommended when releasing particles at high seed densities.

6.3 Sensitivity to Municipal Pumping Rates

Figure 50 illustrates the effect of pumping on the delineation of ESGRAs. Particle tracks were created after adjusting the municipal pumping rates $\pm 10\%$ across the entire model. Overall, the general location of ESGRAs did not change significantly; only slight translations occurred in response to the changing groundwater pumping regime. Specifically, as pumping is decreased, the ESGRAs tend to move further from the stream network, as illustrated in the blue areas of Figure 50.

6.4 Sensitivity to Hydraulic Conductivity Values

Sensitivity to $\pm 10\%$ change in hydraulic conductivity showed similar behaviour as with changing pumping rates: the general location of ESGRAs remained, but they have undergone a slight translation (Figure 51). In this case, the increase in hydraulic conductivity has moved the ESGRAs toward the stream network, similar to that of increased pumping rates. The magnitude of sensitivity to these changes is greater than those observed by varying the groundwater pumping rates by $\pm 10\%$.

6.5 Sensitivity to Groundwater Recharge

Sensitivity to minor changes to the model recharge rates was investigated. Recharge was adjusted $\pm 10\%$ across the model area. Changes in the simulated hydraulic heads were observed within the study catchments; however, there were no appreciable changes to the overall flow patterns within the catchments. As a result, there were no significant changes to the delineated ESGRAs.

7 Conclusions

This report presents the results of the following tasks:

- 1. Review and update of the FEFLOW model in the Barrie, Lovers and Hewitt watersheds;
- 2. Develop a methodology to delineate ESGRAs in a consistent and objective manner;
- 3. Apply the selected methodology to the study area watersheds; and,
- 4. Conduct ESGRA sensitivity and scenario analysis.

7.1 Tier 2 FEFLOW Model Limitations in Relation to the ESGRA Assessment

The Tier 2 model was primarily developed for a subwatershed water balance assessment. While it can be an appropriate tool for establishing the linkage between recharge areas and ecologically significant surface water features its use is subject to some limitations despite the refinements that were undertaken. These include:

- The FEFLOW hydrostratigraphic model is based on a conceptual aquifer model that does not use the conventional stratigraphic names and till mapping developed by the Ontario Geological Survey. The conceptual model may be more appropriate for the deeper aquifers and municipal wellfields. The PRMS recharge model was based on OGS surficial geologic mapping, however. This inconsistency makes refinement of the upper model layers to better represent the shallow subsurface and ESGRA features more difficult. The quality and consistency of the upper model layers and recharge delineation is likely the single most important factor in this assessment.
- The updated model appears to have an improved and more realistic water table configuration. The original model exhibited a number of isolated peaks in the water table, together with a very flat water table through much of the Lovers Creek watershed (despite over 50 m of topographic variation between the main branch and the watershed boundaries). The updated model eliminates the unusual peaks and produced water table levels and gradients that are more consistent with the topography and stream tributary network.
- The model update demonstrates that local refinement can significantly improve the local representation of ecological features and local calibration. Careful selection of boundary conditions is essential.

7.2 ESGRA Methodology and Delineation

This report outlines a methodology for the consistent delineation of Ecological Significant Groundwater Recharge Areas (ESGRAs) based on reverse particle tracking simulations. The

method is based on model assessment, reverse particle tracking, and a standardized cluster analysis algorithm.

The cluster analysis presented here provides an objective means of delineating ESGRAs. The method assumes that endpoint density is representative of flux proportionality occurring at the selected features of interest. The development of the methodology require careful selection of the smoothing parameter (*h*) and the delineation threshold (ε). In this study, the bivariate kernel density estimation was applied to a 25 m uniform grid using a smoothing parameter equal to the grid spacing. The delineation threshold of $\varepsilon = 100$ proved to provide the best results by encompassing a large majority of endpoints in a relatively small area. It is thus recommended that this methodology be followed to ensure consistency with the results presented herein. A clear step-by-step methodology is outlined in Appendix A.

Release point density appeared to work well at uniform distribution of 5 to 10 m. Although nodal release radius showed sensitivity the ESGRA cluster results, this method of particle release is limited to finite element models or possibly just FEFLOW.

7.3 ESGRA Results

The ESGRA results indicate that there is some correlation between SGRA and ESGRA zones, particularly in the west-central portion of Lovers Creek. However, it is apparent that large discrepancies exist between the ESGRAs mapped from particle clusters and the SGRAs mapped in previous efforts (Earthfx, 2010). SGRAs may not be coincident with the ESGRAs mapped from particle clusters because the model used was not designed for this type of analysis and the features of concern (i.e., coldwater reaches, wetlands, etc.) were not explicitly represented in the model. It should also be noted that there appears to be significant cross-watershed boundary flows where recharge occurring within the study area discharges well beyond the study limits; therefore, it would have been more prudent if the ESGRA analysis were conducted as a regional exercise.

7.4 Sensitivity Analyses

The sensitivity analyses presented above have demonstrated that particle tracking results are sensitive to both the method of particle release and model parameter values. Particle density and the use of flux-weighted particle starting points, on the other hand, did not appear to affect particle tracking results. ESGRA results are very sensitive to the location of released particles, and thus it is recommended that a standard methodology be put forward for particle release when dealing with finite-element models where particles are to be released from nodes. The ESGRA cluster analysis from a 50 m nodal release radius created a placement of particles quite distinct from the 25 m release radius, and may be a cause for concern when applying the methods described herein to future projects.

To a lesser degree, the cluster analysis was sensitive to the hydraulic conductivities set in the FEFLOW model. Unlike the case with changing particle release radii, the changes in ESGRA delineation only served to translate the ESGRAs, while preserving the general location of these clusters. Similar results were found for variation is municipal groundwater pumping rates. The ESGRA delineations were found to be insensitive to minor changes in model recharge.

The parameters required to for cluster analysis were investigated. Optimal values were obtained for the study watersheds. Different value of the delineation threshold may be required in different catchments or for different ESGRA scenario.

8 Limitations

Services performed by Earthfx Inc. were conducted in a manner consistent with that level of care and skill ordinarily exercised by members of our technical profession. This report does not exhaustively address all possible conditions that may exist in the study area. Computer models are a simplification of the real world, built from limited and potentially erroneous data, so their results should be considered with care and independently verified. It should be recognized that the passage of time affects the information provided in this report. Environmental conditions can change. Computer simulations are based upon information that existed at the time the data and model was formulated.

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9 References Cited

- AquaResource Inc. and Golder Associates Ltd., 2010, South Georgian Bay West Lake Simcoe Study Area Tier Two Water Budget and Stress Assessment: Draft Final Report: prepared for Lake Simcoe Region Conservation Authority, Nottawasaga Valley Conservation Authority, and the Severn Sound Environmental Association, October 2010.
- DHI-WASY Software, 2011, FEFLOW 6 -- Finite-element subsurface flow and transport system --Installation guide and demonstration exercise.
- Earthfx Inc., 2010, Water balance analysis of the Lake Simcoe basin using the Precipitation-Runoff Modelling System (PRMS). Report prepared for the South Georgian Bay-Lake Simcoe Source Protection Region.
- Golder Associates and AquaResource Inc., 2009, Nottawasaga Valley Conservation Authority water budget model – Geological/hydrostratigraphic model development -- Interim Report: prepared for the Nottawasaga Valley Conservation Authority and Lake Simcoe Conservation Authority.
- Leavesley, G.H., Lichty, R.W., Troutman, B.M., and Saindon, L.G., 1983, Precipitation-Runoff Modeling System: User's Manual: U.S. Geological Survey Water Resources Investigations Report 83-4238, 207 p.
- Nottawasaga Valley Conservation Authority, 2010, Report on the HSPF Model -- NVCA and SSEA Watersheds (Draft).
- USEPA, 1997, Hydrological Simulation Program FORTRAN (HSPF) Version 11.0 User's manual for Release 11.
- Wand, M.P., M.C. Jones, 1993. Comparison of smoothing parameterizations in bivariate kernel density estimation. Journal of the American Statistical Association 88. pg. 520–528.

TABLES

Subwatershed	Watershed Area (km²)	Applied Surface Recharge ¹ (PRMS Model) (m ³ /day)	Stream leakage to Groundwater System (Injection nodes) (m³/day)	Groundwater discharge to stream network (m³/day)	Stream leakage (injection nodes) as a percent of Applied Surface Recharge.
Barrie Creeks	37.5	16,500	850	1.92	5.1%
Lover's Creek	59.9	22,700	12,500	15,270	67.2%
Hewitt's Creek	17.5	5,980	393	352	6.5%

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Table 1: Summar	y of Water In	jection Node FI	ows: Barrie, I	Lovers and Hewitts	Creek Watersheds

Notes:

1: The applied groundwater recharge was determined from the distributed PRMS model based on surficial geology, land cover and climate inputs as simulated. The distributed (spatially variable) cell based estimate of recharge was applied to the FEFLOW elements. The number is in this column represents the total recharge applied to the catchment.

Table 2: Percent of endpoints released from all features covered by ESGRAs with varying smoothing parameter (*h*) and delineation threshold (ε). Of the 231,776 points release, only 166,050 remained in the study area or had travel times greater than 1 day.

1/ε	h = 25	h = 50	h = 100	h = 200
0.001	100.0%	100.0%	100.0%	100.0%
0.005	98.9%	99.5%	99.7%	99.9%
0.01	96.7%	98.7%	99.2%	99.6%
0.05	74.8%	85.0%	87.1%	92.7%
0.1	48.0%	68.0%	69.1%	78.0%

Table 3: Percent of watershed area covered by ESGRA.

1/ε	h = 25	h = 50	h = 100	h = 200
0.001	27.7%	40.6%	57.8%	79.6%
0.005	19.7%	31.3%	46.5%	68.6%
0.01	15.3%	25.8%	39.2%	60.8%
0.05	5.3%	10.9%	17.3%	34.1%
0.1	2.0%	5.4%	8.4%	18.5%

FIGURES



Figure 1: The SGB-WLS Tier 2 study area and location of the Barrie, Lovers, and Hewitt Creek subwatersheds (Map from AquaResource and Golder, 2010).



Figure 2: Location of significant groundwater recharge areas (SGRA) in the Barrie, Lovers, and Hewitt Creek subwatersheds (based on data from Earthfx, 2010).



Figure 3: The model mesh in the vicinity of the study area



Figure 4: Comparison of the simulated streams versus the actual stream network. (Model = purple, MNR mapping = Blue). For Barrie creeks, please see Figure 5.



Figure 5: Comparison of the simulated streams versus the actual stream network in the Barrie creeks watershed. (Model = purple, MNR mapping = Blue).



Figure 6: Simulated heads in Layer 1 in the Barrie Creeks area (land surface topography ranges from 220 to 236 masl). See Figure 7 for the location of inset.


Figure 7: Comparison of the simulated stream network and wetland locations (modelled streams shown in purple). Red rectangle denotes inset for Figure 6.







Figure 9: Comparison of the simulated stream network and brook trout and sculpin capture sites (modelled streams shown in purple).

Earthfx Inc.



Figure 10: Estimated groundwater recharge in the study area. Wetland areas were assumed to be groundwater discharge zones and were modelled as having zero recharge

Model Layer	West (Niagara Escarpment)	Central (NVCA & West LSRCA)	North East (Severn Sound)
1	SC1 (Confining Subunit of A1)		Drift (0-5m)
2	SA1 (Aquifer Subunit of A1)		
3	SC2 (Confining Subunit of A1)		
4	SA2 (Aquifer Subunit of A1)		
5	SC3 (Confining Subunit of A1)		
6	SA3 (Aquifer Subunit of A1)		
7	SC4 (Confining Subunit of A1)		
8	SA4 (Aquifer Subunit of A1)		
9	Guelph Amabel	C1	
10		A2	
11		C2	
12	Clinton Cataract	A3	
13		C3	
14	Queenston	A4	
15		C4	
16	Georgian Bay		Precambrian
	Bottom slice of layer 16 represents top of Simcoe Group		

Figure 11: Tier 2 model layers



Figure 12: Tier 2 geologic model.



Figure 13: Tier 2 hydrostratigraphic model.



Figure 14: Stream leakage to/from the groundwater system.

Legend:

- Discharge from the groundwater system to streams: scaled green to blue symbols
- Leakage from the streams to groundwater ("injection nodes"): scaled orange to red

Figure 14 shows the position of the "injection nodes" (red circles colour scaled to injection rate) positioned at the headwaters of many of the tributaries. At these nodes the model is injecting significant quantities of water. The injection node flux in Lover's creek is equal to 67% of applied groundwater recharge.

The groundwater injection nodes generally occur at the headwaters of the smaller tributaries. Headwater streams, in reality, are usually small intermittent tributaries or springs (groundwater discharge points), and not significant recharge points. There is no known field evidence to suggest that the small headwater tributaries are significant sources of groundwater recharge.



Figure 15: Cross section sketch showing how constant heads inject water below Lovers Creek.



Figure 16: 3-D view of Lover's Creek, looking north towards Kempenfelt Bay. Ground surface is shown in grey. Areas where the model predicted water table elevation is above ground surface are shown in blue-green.



Figure 17: Areas where simulated groundwater levels are above ground surface.



Figure 18: Sketch showing how simulated heads above land surface affect backward tracking.



Figure 19: Sketch showing why anomalously high heads occur in the Barrie Creeks area.



Figure 20: Added and corrected stream reaches



Figure 21: Cauchy boundary conditions added to represent wetlands (Mapped wetlands = light green, Cauchy wetland element nodes = dark green)



Figure 22: Original and Adjusted K in Layer 1



Figure 23: Original and Adjusted K in Layer 2



Figure 24: Original and Adjusted K in Layer 3



Figure 25: Original and Adjusted K in Layer 4



Figure 26: Original and Adjusted Vertical Hydraulic Conductivity in Layer 1



Figure 27: Original and Adjusted Vertical Hydraulic Conductivity in Layer 2



Figure 28: Original and Adjusted Vertical Hydraulic Conductivity in Layer 3







Figure 30: Simulated heads in upper layer, revised model calibration.



Figure 31: Simulated heads in upper layer, Tier 2 model.



Figure 32: Screenshot of FEFLOW reverse particle tracking from Lovers Creek, with recharge.



Figure 33: Sample particle release radius around a single stream node.



Figure 34: Sample 10 m grid distribution of wetland release particles.



Figure 35: Sample release points for coldwater reaches and fish capture areas. A $200x400 \text{ m}^2$ buffer area is place over the points of interest and a 5 m grid of particles are released within these buffer areas.















Figure 39: ESGRAs defined by backward tracking from coldwater stream reaches.



Figure 40: ESGRAs defined by backward tracking from wetlands and coldwater reaches combined.







Figure 42: Final ESGRAs defined by backward tracking from all features. All particle endpoints are shown including those classified as outliers and those with travel time less than 1 day.



Figure 43: Forward particle tracking from study subcatchment showing cross-watershed flow.



Figure 44: Forward tracking of particles from the ESGRAs of all features (Figure 41).



Figure 45: Forward tracking of particles from SGRAs. (Note that the delineation threshold was increased to $\varepsilon = 1,000$ to produce this figure)



higher).



Figure 47: ESGRA results using a particle release density of 50 particles per node (from 4th order streams or higher).



Figure 48: Flux-weighted backward tracking from streams, 100 particles per node (from 4th order streams or higher).


Figure 49: Flux-weighted backward tracking from streams, 100 particles per node (from 4th order streams or higher).



Figure 50: Backward tracking sensitivity to changes in groundwater pumping (from 4th order streams or higher).



Figure 51: Backward tracking sensitivity to changes in hydraulic conductivity (from 4th order streams or higher).

10 Appendix A: ESGRA Delineation Methodology

The following section provides a brief description on the methods used to delineate Environmentally-Significant Groundwater Recharge Areas (ESGRAs). The methods outlined here were developed for the Barrie, Lovers, and Hewitts Creek ESGRA assessment and are based on techniques that were optimized to develop a consistent, unbiased, and technically sound methodology that can be applied consistently in future studies in the other subwatersheds.

10.1 Reverse (Backward) Particle Tracking

Distributed long-term average recharge from a surface water model is applied as input to a calibrated groundwater model. The steady-state groundwater fluxes determined by the model are used to create a velocity field. Virtual particles released from environmentally sensitive features (such as coldwater streams, wetlands, or spawning sites) are then tracked back in to their point or origin. Where the particles intersect land surface defines their point of entry to the groundwater system and are defined as particle *endpoints*.

10.2 Particle Endpoint Cluster Analysis (Theory)

Typically, endpoints tend to cluster in areas of high recharge, while areas of lower recharge may end up with individual or small groups of particles. Discriminating between endpoints belonging to a cluster and isolated particles (outliers) can be subjective. For the purpose of this study, "clusters" are defined as areas with a *relatively* high density of particle track endpoints; all endpoints that exist outside of the clusters are considered outliers and are rejected. The delineated clusters are then deemed to represent ESGRAs based on the assumption that the density of particle track endpoints correlate to recharge areas that are significant to sustaining environmentally sensitive features.

A method was developed to objectively evaluate endpoint clusters to delineate ESGRAs for the Barrie, Lovers, and Hewitts ESGRA study. The method proposed was adopted from published, peer-reviewed methodologies. This technique was further tested and refined so that it can be applied to other subwatersheds ensuring that the delineation of ESGRAs across the LSRCA can be conducted in a consistent manner.

The method is based on *multivariate kernel density estimation* (Wand and Jones, 1993), and is defined by:

$$\hat{f}_{H}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} H(\mathbf{x} - \mathbf{x}_{i})$$

where

x is a point in space (i.e., for the bivariate case, it would be defined by the coordinates *x* and *y*; that is x = (x, y)

- X_i is the coordinate of a point of interest (in this case would be the particle track endpoints), that is, $X_i = (x_i, y_i)$;
- n is the total number of endpoints;
- K_H is the scaled kernel multivariate function, based on the standard bivariate normal (Gaussian) kernel, where

$$_{H} (\mathbf{x}) = \begin{bmatrix} 2\pi & |\mathbf{H}| & |\frac{1}{2}\mathbf{\hat{x}} & \mathbf{H} & (\frac{1}{2}\mathbf{x}) \end{bmatrix}^{-1},$$

where

h

Η

is the bandwidth matrix – assumed here to be symmetrical, thus $H = [{}^{h} Q; 0 h]$ and, is a smoothing parameter (analogous to the normal standard deviation).

10.3 Why the Chosen Cluster Methodology?

It is acknowledged that simpler and possibly more intuitive approaches to point cluster density analysis exist; however, there are limitations that are overcome when using the bivariate kernel density estimation. The simplest approach would involve overlaying a grid on the map of endpoints and counting the number of particle endpoints within each grid cell. This is known as the *histogram approach*. As illustrated using the one-dimensional case, it can be seen that the choice of origin affects the density distribution estimate (where density is determined by counting the number of endpoints per histogram bin). Two histograms (red and grey) were produced from the random set of points lying on the x-axis of Figure 52, illustrating the relative frequency of points clustering within bins of size 0.1 (these bins are analogous to grid cells in the two-dimensional case). Depending on the origin of the histogram (0 for the grey and 0.5 for the red), cluster analysis performed using the histogram approach resulted in a different density approximation. The histogram approach is also dependent on the bin size, and would yield different endpoint density distribution for each grid or bin size.



Figure 52: Inconsistent density estimation using the histogram approach.

The bivariate kernel density estimation methodology avoids the inherent bias and non-uniqueness of the simple histogram approach. The kernel density estimation creates a continuous histogram independent of grid size, origin, and grid orientation. A one-dimensional example is shown in Figure 53.



Figure 53: Sample kernel density estimation compared with the histogram.

Here, the one-dimensional sample kernel density estimation function is the sum of multiple univariate Gaussian distributions surrounding every random point lying on the x-axis. The function provides a smoothed estimate for a density distribution that is invariant to the choice of origin or bin size. The method can be extended to two dimensions to derive a density distribution independent of grid origin, orientation, and cell size, as discussed below.

10.4 Particle Endpoint Cluster Analysis (Application)

The distance between an arbitrary point vector \mathbf{x} (located by the coordinates (x, y)) and a particle endpoint \mathbf{X}_i (X_i, Y_i) along a straight path is equal to $d_i = ||\mathbf{x} - \mathbf{X}_i|| = \sqrt{(x - X_i)^2 + (y - Y_i)^2}$. (vectors have been denoted using bold text.) Assuming kernel mass to be spherically symmetrical, the scaled kernel bivariate function can be simplified to:

$$_{H}$$
 (*d*_{*i*}) = $[2\pi (h_{h}^{2})^{2}e]^{2}$,

and thus the bivariate kernel density estimation becomes:

$$\hat{f}_{H}(x,y) = \frac{1}{2\pi nh^{2}} \sum_{i=1}^{n} e^{-\frac{1}{2} {\binom{d}{h}}^{2} 9}.$$

The above equations require the choice of two parameters: the smoothing parameter (h), which is analogous to the standard deviation of the bivariate distributions and effectively represents the

"spread" or "reach" at which an endpoint has an influence on the density surface; and the delineation threshold (ε), which is used to remove areas of relatively low particle endpoint density.

Figure 54 illustrates the smoothing parameter's effect on cluster delineation. In this figure, cluster analysis was performed on a sample set of reverse particle track endpoints (Figure 54a) for different values of the smoothing parameter evaluated on a 25 m uniform grid, where the bivariate kernel density estimation is evaluated at the grid cell centroids.

First, a smoothing parameter smaller than the grid cell size (at h = 10 m) was evaluated to demonstrate that the smoothing parameter has a lower limit equal to the resolution of the distributed kernel density estimation (Figure 54b). It is apparent that this choice of h is a poor choice for the task delineating clusters because cells with only one particle endpoint can be classified as either a cluster or an outlier, just based on the distance of the point to the centroid of the grid cell. While the method successfully identified areas of clustered endpoints, it performed no better than simply identifying cells that contain more than one particle, (i.e., the histogram approach).

Figure 54c shows the density field when the smoothing parameter was set to the grid cell size (h = 25 m). In this case, problems identified in the previous case were remedied. The method properly identified areas of relatively high density, while avoiding endpoints that should be considered as outliers. The range in density values, as shown by the colour scale, also become more apparent than in the previous case. Cluster delineation is also much more contiguous (compared with h = 10 m) which will help in mapping ESGRAs.

Doubling the smoothing parameter (h = 50 m) served to expand the extent of the higher density regions slightly beyond the locations of the particle endpoints (Figure 54d). This method may become problematic as it now includes areas where no endpoints exist at all. While it is possible to increase the delineation threshold (ε – to be described below) to exclude particle-free areas, doing so ignores areas that are dense but distributed in a more linear fashion (such as the 'trail' of points directed to the northwest at the top of the figure). For example, if the threshold is chosen such that all areas shown in light blue are rejected, many regions of this sample point distribution will be incorrectly classified as non-clusters. One benefit of note, is that the densest areas have become increasingly distinct, showing more green, yellow, and red colourations around areas where endpoint density is obviously highest.

With an even larger smoothing parameter, where h = 100 m, the bivariate kernel density estimation extends the delineation farther into regions with little or no point density (Figure 54e). Another apparent issue is that the regions indicating high density begin to take a more circular form, thus departing from the shape of the cluster distributions. This choice of smoothing parameter still isolates individual endpoints and rejects them as part of the ESGRA.

The final three cases, h = 250, 500, and 1000 m, are presented for illustrative purposes only. Clearly, smoothing parameters at these scales only describe general/global areas of particle density and fails to identify individual clusters (Figure 54f, g, and h) to a point where at h = 1000 m the density field become circular and shows no apparent form whatsoever.



Figure 54: effect of smoothing parameter (h) on the delineation of spatial density

Legend: a: original point distribution; b: h = 10m; c: h = 25m; d: h = 50m; e: h = 100m; f: h = 250m; g: h = 500m; h: h = 1000m. $\varepsilon = 100$.

<u>Delineation threshold(ε)</u>: To reject areas of the bivariate kernel density distribution based on *relatively* low densities, the density surface is normalized by dividing all kernel density values by the maximum estimation ($\hat{f}_{H,max}$). A cluster is defined by the selected threshold density (ε) where:

$$\hat{f}_H(x,y) > \frac{\hat{f}_{H,max}}{\varepsilon}.$$

For example, $\varepsilon = 100$ means that all areas with an evaluated density less than 1% of the highest density would be considered as outliers. The delineation threshold parameter may need adjustment based on the particle endpoint scenario, and a good approach to fine-tuning this parameter would be to compare cluster area to the number of endpoints contained within these areas.

10.5 Recommended Methodology and Control Parameters

The cluster analysis presented here provides an objective means of delineating ESGRAs. The method assumes that endpoint density is representative of the proportion of flux occurring at the selected features of interest. The development of the methodology requires careful selection of the delineation threshold (ε). The bivariate kernel density estimation was evaluated on a uniform 25 m grid/raster and a smoothing parameter (h) chosen for the pilot study was 25 m and corresponded to the grid size.

The bivariate kernel density estimation algorithm presented here can be made more computationally efficient if a maximum evaluation distance (d_{max}) is set. The maximum evaluation distance was set to three times the length of the smoothing parameter and all evaluation distances where $(d_i < d_{max} = 3h)$ were rejected, implying that evaluations will be kept within three standard deviations from the center-mean of the scaled kernel bivariate function.

A step-by-step methodology is presented below:

- 1. Perform reverse particle tracking and locate the coordinates where every pathline intersects ground surface and consider these "particle endpoints."
- 2. Using a 25 m raster, determine the distance (d_i) between grid cell centroid and endpoints *i* determined in step 1.
- 3. For all distances from an endpoint to the grid centroid (d_i) that are less than or equal to 3h, where h = 25 m, evaluate the scaled density estimator $\hat{f}_H(x, y)$, using:

$$\hat{f}_{H}(x,y) = \frac{1}{2\pi n h^{2}} \sum_{i=1}^{n} e^{-\frac{1}{2} \left(\frac{d}{h}\right)^{2}}.$$

- 4. Repeat the above steps for every grid cell.
- 5. Determine $\hat{f}_{H,max}$ (the highest evaluated scaled density estimation evaluated) and normalize all values by dividing by $\hat{f}_{H,max}$. (so that the normalized $\hat{f}_{H,max} = 1$.)
- 6. Select an appropriate delineation threshold (ε) and reject all \hat{f}_H that are less than $\frac{1}{\varepsilon} \hat{f}_{H,max}$. ($\varepsilon = 100$ was used in the pilot study)
- 7. The remaining density estimations, where $\hat{f}_H > \frac{1}{\epsilon} \hat{f}_{H,max}$, are then classified as ESGRAs.