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Technical Memorandum

Reference # 12985.101

Status: Correspondence

2nd August 2018

Attention:	**Reed Harris**
CC:	Rob Nairn
From:	Alex Brunton

RE: Lake Melville Model Setup and Results

Summary

Two numerical simulation models were used to predict the downstream fate of methylmercury (MeHg) generated in the Muskrat Falls Reservoir flood zone. A high-resolution hydrodynamic model of Goose Bay and Lake Melville was applied using the Delft3D model to examine the effects of downstream mixing and dilution. An associated box model was created to further account for losses due to photodegradation and settling. The models used five-year predictions of excess MeHg entering the lower Churchill River following reservoir filling. These predictions were based on two estimates of the reservoir flood zone signal: (1) Predictions from a mechanistic model (ResMerc) and (2) estimates derived using field data from the FLUDEX experiment in the Experimental Lakes Area in Ontario. Both estimates were developed by Reed Harris Environmental Ltd (Harris and Hutchinson, 2018). Results of simulations using the two loading estimates were averaged for the final analysis.

Area-weighted changes in MeHg concentrations over time were critical to understand the nature and duration of exposure by aquatic biota over and above baseline concentrations to estimate exposure to MeHg in a post-inundation situation. Predicted increases in water column MeHg concentrations declined with distance from the reservoir, due to the effects of dilution, photodegradation and settling. The creation of Muskrat Falls Reservoir was predicted to increase MeHg concentrations in the top 20 m of the water column by 0.019 ng/L in Goose Bay (maximum 3-year average increase in concentration), and 0.005-0.006 ng/L in Lake Melville. MeHg concentrations were predicted to increase less at depths below 20 m: by up to 0.013 ng/L in Goose Bay, and 0.002-0.003 ng/L in Lake Melville. In the top 20 m of the water column, the predicted relative increase over the baseline concentration of 0.017 MeHg was approximately 2x in Goose Bay and 1.3-1.4x in Lake Melville.

Outline

The memorandum includes the following sections:

1. Hydrodynamic Model Overview
2. Summary of Hydrodynamic Model Setup and Calibration
3. Summary of Hydrodynamic Model Results
4. Box Model Overview
5. Box Model Setup and Calibration
6. Box Model Results

Hydrodynamic Model Overview

Delft3D is a three-dimensional hydrodynamic model with wave, sediment transport (cohesive and non-cohesive) and water quality modules. Delft3D was developed by Delft Hydraulics in the Netherlands, and it is a non-commercial, open-source model, which is an important consideration for public agencies. Delft3D is widely considered to be one of the best available models for the prediction of flow and particle fate, particularly in estuarine conditions.

The three-dimensional version of Delft3D model uses a curvilinear grid system, which fits the shoreline boundary conditions in the Lake. Delft3D-FLOW is the hydrodynamic component of the Delft3D model suite, and it can be applied to a wide range of applications, including:

- Tide and wind-driven flow resulting from space and time-varying wind and atmospheric pressure
- Density driven flow and salinity intrusion
- Horizontal and vertical transport of matter on large and small scales
- Stratification in seas, lakes and reservoirs
- Small scale current patterns near harbor entrances

The primary purpose of Delft3D-FLOW is to solve various time-dependent, non-linear differential equations related to hydrostatic and non-hydrostatic free-surface flow problems on a structured orthogonal grid. The equations solved are mathematical descriptions of physical conservation laws for:

- Water volume (continuity equation)
- Linear momentum (Reynolds-Averaged Navier-Stokes (RANS) equations)
- Tracer mass (transport equation), e.g., for salt, heat (temperature) and suspended sediments or passive pollutants

Several different datasets are necessary to set up the hydrodynamic model:

- Coastline and bathymetric data for the Lake and the adjacent areas
- High resolution aerial imagery – used to delineate the lake boundary
- Tide elevations and river flow data in the study area
- Temperature and salinity conditions at the model boundaries
- Amount of excess MeHg entering the Lake system

These datasets are discussed in the subsequent sections of this memorandum.

Summary of Hydrodynamic Model Setup and Calibration

Where available, empirical, site-specific information as possible was used (e.g., river discharge, bathymetry, shoreline data, etc) to construct the Delft3D model, so that it represents the site-specific conditions in the study area as much as possible.

Coastline Data

Coastline data are necessary to define the Delft-3D model domain. The coastline in the study area was digitized from Google Earth and converted for import to the Delft3D model.

Model Grid

The model computational grid was set up to achieve a balance between having sufficient resolution in the narrow sections of the domain, while avoiding over-refining the grid, which would result in an unacceptably-long computation time for the model runs. Overall, there were 18,500 active grid cells in the horizontal plane, and up to 17 layers deep in the vertical direction. Due to limited data for the lower Churchill River, a simplified representation of the river was developed upstream from Goose Bay. This stretch of river was used to define the main inflow to Goose Bay and it was outside the main area of interest, so this simplification was appropriate for determination of flows within the lake itself. The grid cell resolution in the lower Churchill River was 9 cells across the width of the river (each cell was ~100-300 m wide), and the cells were oriented in the dominant downstream flow direction. The river portion of the domain extended approximately 21 km upstream from the entrance to Goose Bay. The grid cell size in the Narrows was approximately 250 m x 250 m, with a minimum of 4 cells across the Narrows, and the average grid cell size in Lake Melville was 750m x 750m. Figure 1 shows the final model grid.

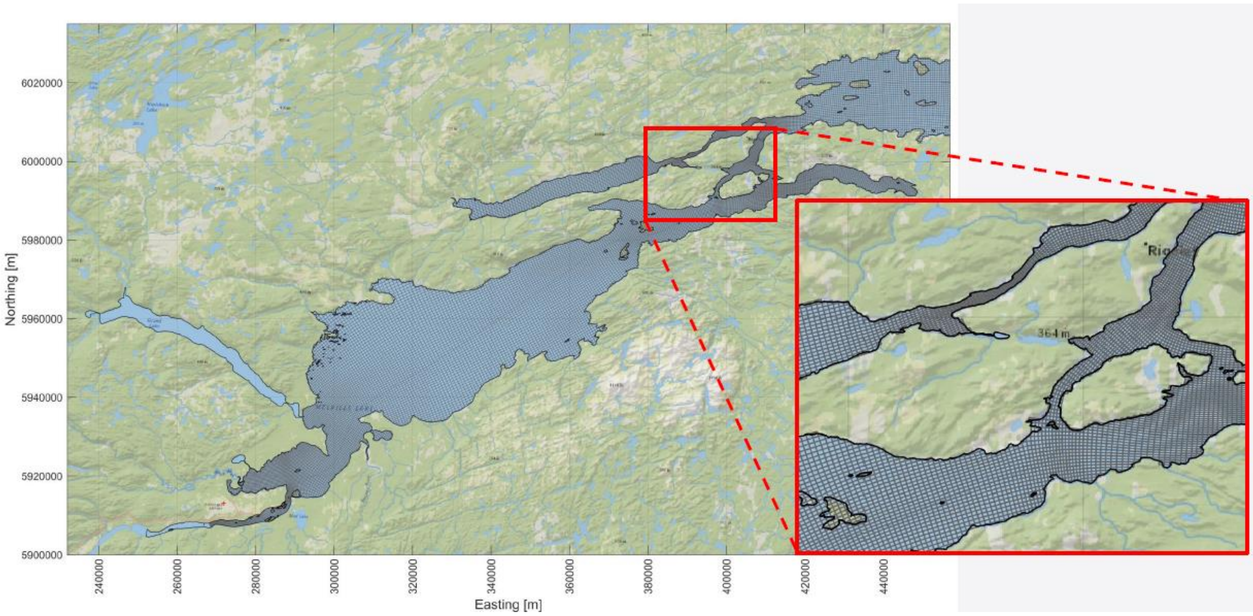

Figure 1 Hydrodynamic Model Grid

Hydrodynamic Model Bathymetry

Model bathymetry was derived from Canadian Hydrographic Survey charts for Lake Melville and then adjusted to mean sea level in the area. Figure 2 shows the final model bathymetry.

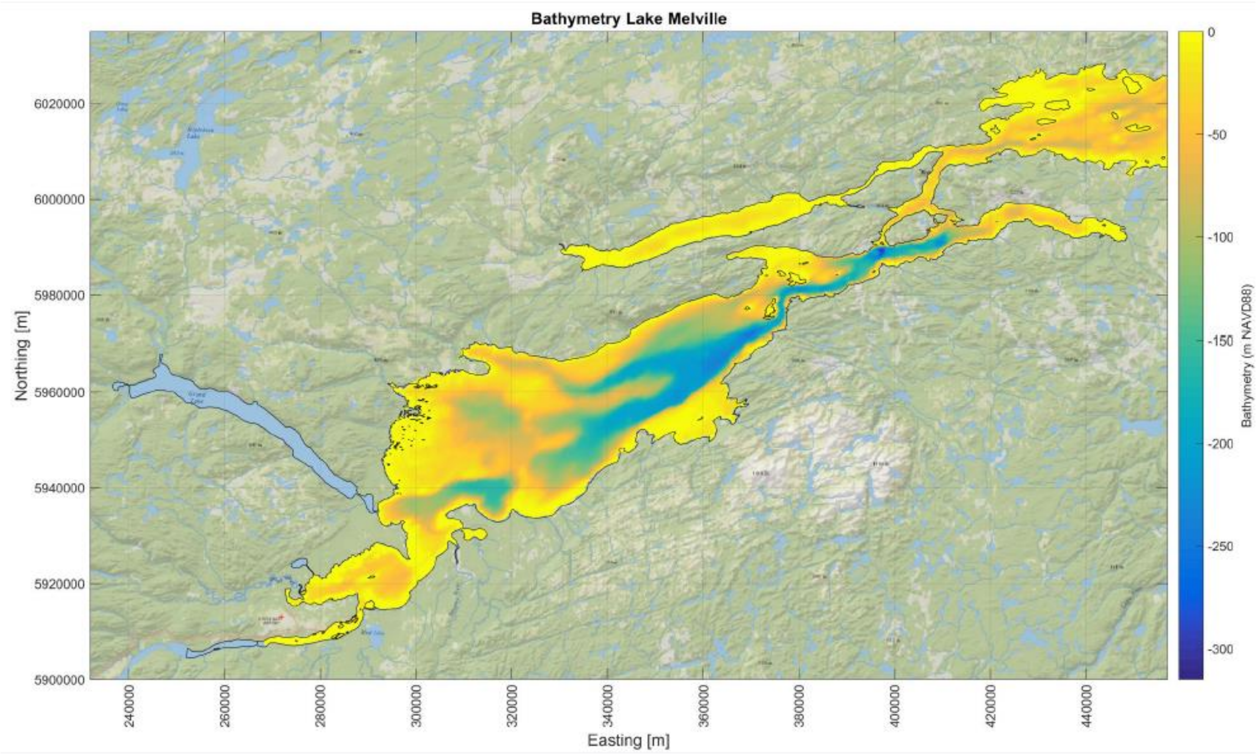

Figure 2 Hydrodynamic Model Bathymetry

Model Atmospheric Conditions

Atmospheric data were downloaded from the Government of Canada Historical Climate Data website[1] for the station at Goose Airport, Goose Bay. This is an hourly dataset, including: temperature (Celsius), relative humidity (%), wind direction (10's deg), wind speed (km/h), visibility (km), atmospheric pressure (kPa) and Cloudiness (%). The data were available for 2010-2017. Gaps in the wind speed and direction data were replaced with zero values.

[1] http://climate.weather.gc.ca/climate_data/

Model Boundary Conditions

Ocean Water level

The water level at the ocean boundary used the astronomic constituents supplied by Wood PLC.[2] Baird compared the water level time series in the model to predicted levels by DFO and determined that the Wood constituents were adequate for use in the model study.

Ocean Temperature and Salinity

Baird retrieved temperature and salinity data for transects at Seal Island, NL, from the DFO Marine Environmental Data Section (MEDS) Portal.[3] A constant temperature of 1 degree Celsius has been used for the Ocean Boundary. This is a reasonable assumption based on data retrieved for Seal Island. Salinity was set to 32 ppt, decreasing to 24 ppt in the top 5 layers. This was based on the data retrieved from Seal Island and the salinity measurements at M2 retrieved from a Memorial University Report.[4]

Lower Churchill River Discharge

Discharge data for the Lower Churchill River were downloaded from the Environment Canada historical hydrometric data portal[5] for station 03OE001 (Churchill River Above Upper Muskrat Falls) for the period 2010-2015. The gauge is located approximately 45 km upstream from where the lower Churchill River enters Goose Bay. This is approximately 20 km upstream from the model boundary in the lower Churchill River. The model assumed no additional inflows in this section and the flows from Muskrat Falls were transposed to the Delft3D upstream boundary. Water temperatures in the lower Churchill River were calculated based on available air temperature data ($T_{water} = 5.0 + 0.75*T_{air}$).

Watershed Inflows

The inflows for rivers other than the lower Churchill River account for approximately 20% of freshwater inflow to Lake Melville, and they are ungauged. The freshwater inflow discharges from the tributary watersheds to Goose Bay and Lake Melville were calculated using an area-weighted method (compared to the lower Churchill River watershed). The watersheds were delineated from the digital terrain model of the area, including a 'burn-in' of the streamlines from the NHD streamline dataset (Figure 3). Water temperatures in the watershed inflows were calculated based on the same air temperature relationship as for the lower Churchill River ($T_{water} = 5.0 + 0.75*T_{air}$). Except for the lower Churchill River, which was modelled explicitly, point sources have been used to represent the watershed inflows to the hydrodynamic model.

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[2] Wood PLC, 10 April 2018, pers. comm.
[3] http://www.isdm.gc.ca/isdm-gdsi/azmp-pmza/hydro/index-eng.html
[4] Lu, Z., DeYoung, B. and Banton, S. 2014. Analysis of Physical Oceanographic Data from Lake Melville, Labrador, September 2012 - July 2013. Memorial University Physics and Physical Oceanography Data Report 2014, I.
[5] https://wateroffice.ec.gc.ca/download/index_e.html?results_type=historical

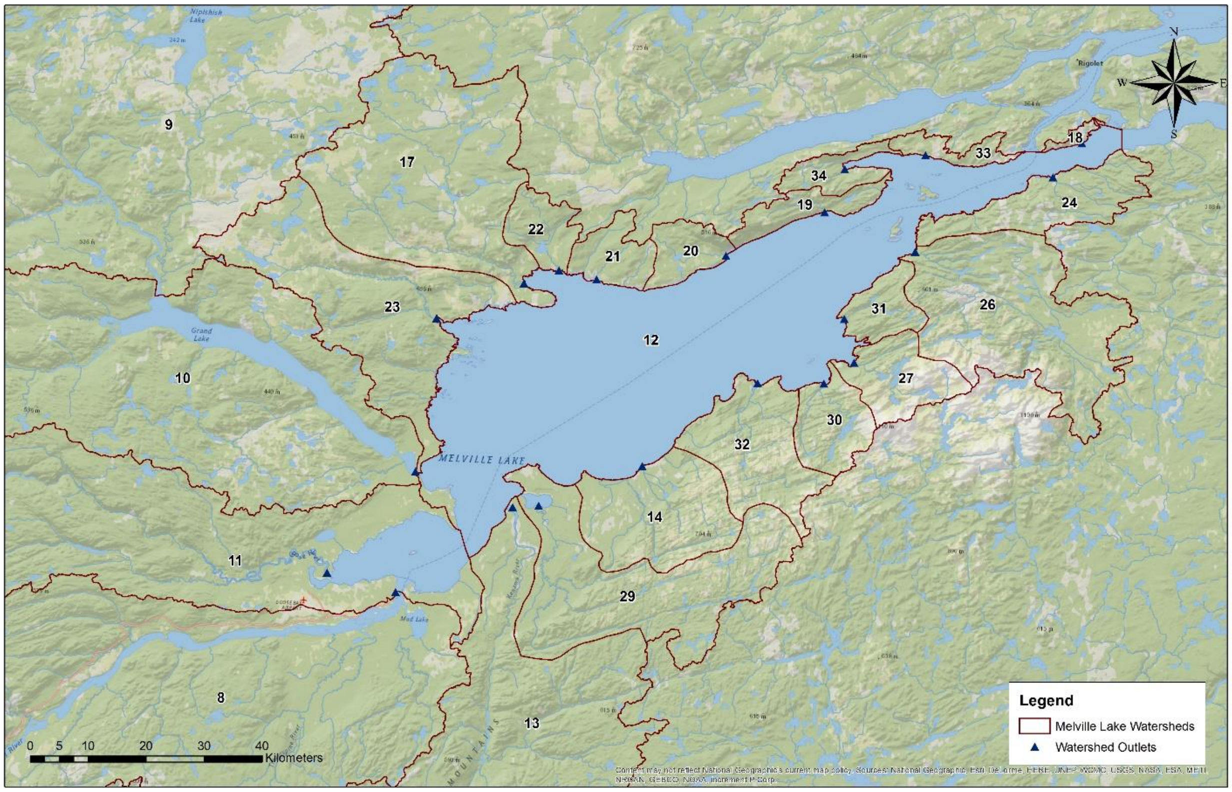

Figure 3 Watersheds discharging to Goose Bay and Lake Melville

Excess MeHg Load from Muskrat Falls Reservoir

Here we define excess MeHg as the increase in load or concentration above baseline, associated with flooding in Muskrat Falls Reservoir. The overall load or concentration is the baseline plus the increase.

Predictions of excess MeHg concentrations and loads exported from Muskrat Falls Reservoir were provided by Reed Harris Environmental Ltd. to Baird (Figure 5). Two sets of excess concentration predictions were provided: one from the output of the ResMerc model, and one based on empirical data from the Experimental Lakes Area FLUDEX experiments (see Harris and Hutchinson, 2018). Both estimates spanned the first 5 years after flooding, a period during which the reservoir MeHg loads and predicted downstream concentrations in water both peaked and began to decline. These predictions were initially applied as a conservative tracer in the Delft3D model. Subsequent simulations using a box model also considered the effects of photodegradation and settling.

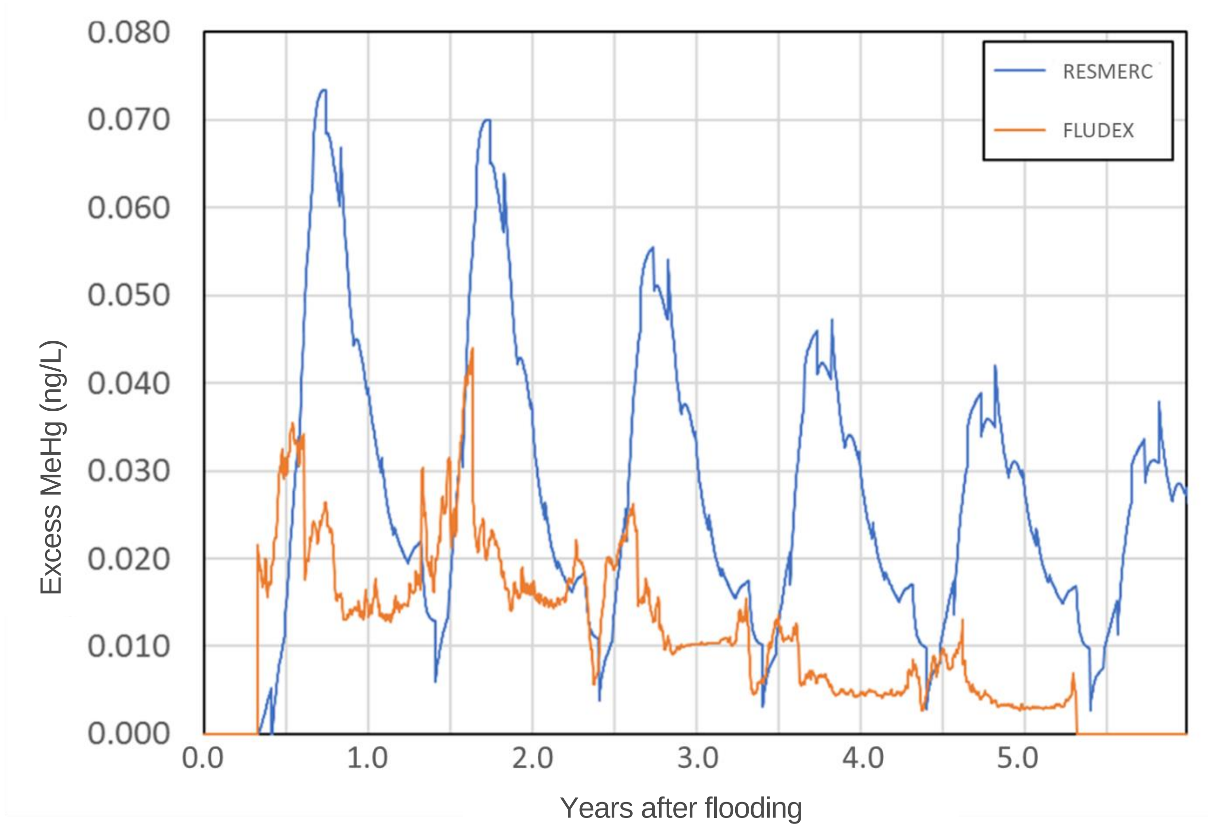

Figure 4 Excess MeHg inflow concentrations (above baseline) based on loads from the ResMerc simulations and the FLUDEX experiments (Harris and Hutchinson, 2018), and flows in the lower Churchill River. Note: Flooding begins in May of first year.

Hydrodynamic Model Calibration

Temperature, Salinity and Density

Comparisons between digitized measurements presented in the Memorial University report for the period in August-October 2012 and model results were made. Overall, modelled temperature, salinity and density profiles showed the same trend as the measurements with respect to the epilimnion, thermocline and the hypolimnion at the Memorial Sonde (conductivity, temperature and pressure (depth) also known as 'CTD probe') locations (Figure 5). Figure 6 to Figure 8 show examples of measured-modelled comparisons on individual days. A good comparison in the upper layers for all 3 parameters is observed. In the deeper layers, temperature is slightly overpredicted, whereas salinity and density are slightly underpredicted.

Model performance statistics are summarized in Table 1 for the final calibrated model. The performance statistics show:

- Water temperature predictions were strongly correlated[6] with observations, and model skill[7] for temperature was high. Modelled values were generally within 3 ^{o}C of observed values, with modelled temperature being warmer than observed.
- Water salinity predictions were strongly correlated with observations, and model skill for salinity was high. Modelled values were generally within 3 ppt of observed values, with modelled salinity being slightly lower than observed.
- Water density predictions were strongly correlated with observations, and model skill for density was high. Modelled values were generally within 2 kg/m^3 of observed values, with modelled density being slightly lower than observed.

The model performance is considered appropriate for determining the distribution and changes in the above parameters. Further calibration of the model may improve the match between measured and predicted parameters, although additional field data would be required to undertake this.

[6] Quantified using the Pearson product-moment coefficient, R

[7] The skill score is an index of agreement between measured and modelled values (Willmott, 1981). A skill score >0.8 is considered excellent.

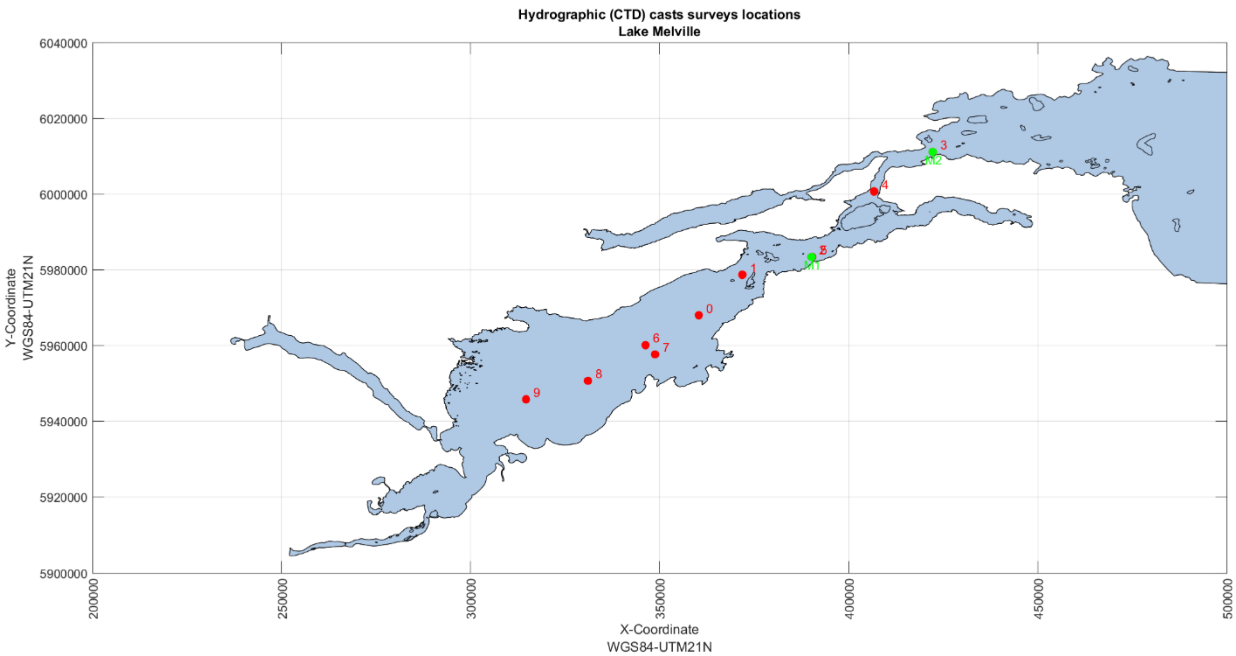

Figure 5 Locations of CTD cast measurements from the Memorial University report. Red dots show the location of CTD probe profiles and Green dots (M1, M2) show the location of Acoustic Doppler Current Profiler (ACDP) deployments

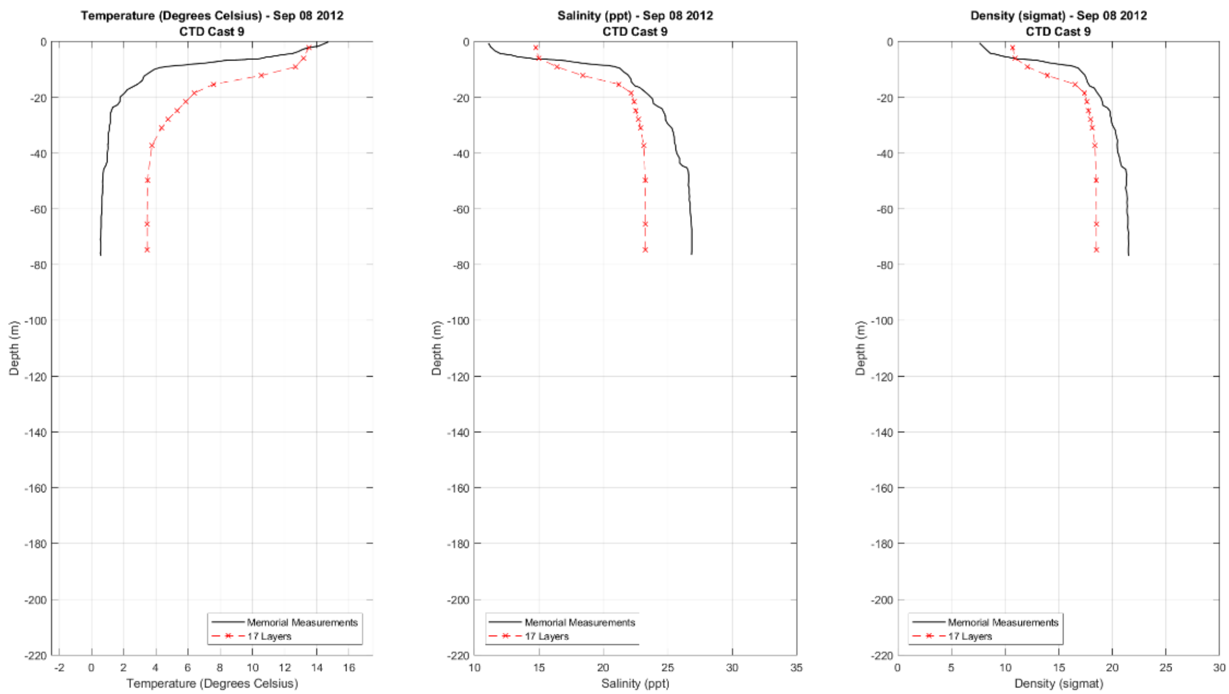

Figure 6 Comparison of measured-modelled temperature, salinity and density in west Lake Melville (CTD9)

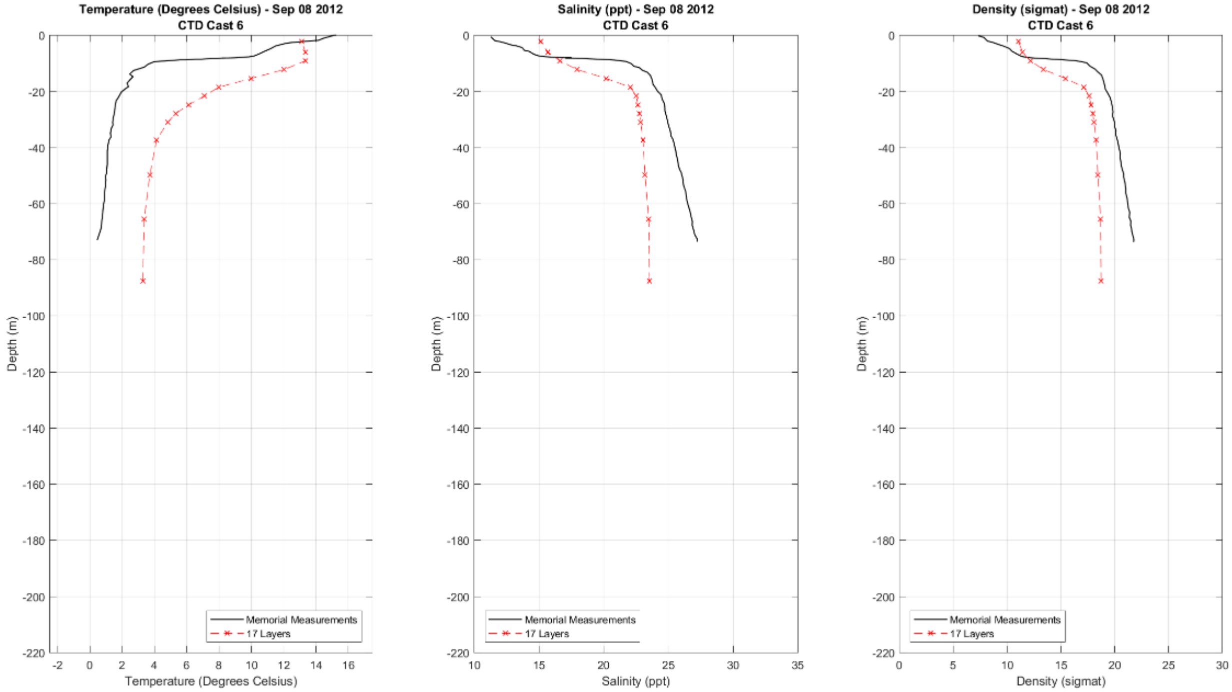

Figure 7 Comparison of measured-modelled temperature, salinity and density in central Lake Melville (CTD6)

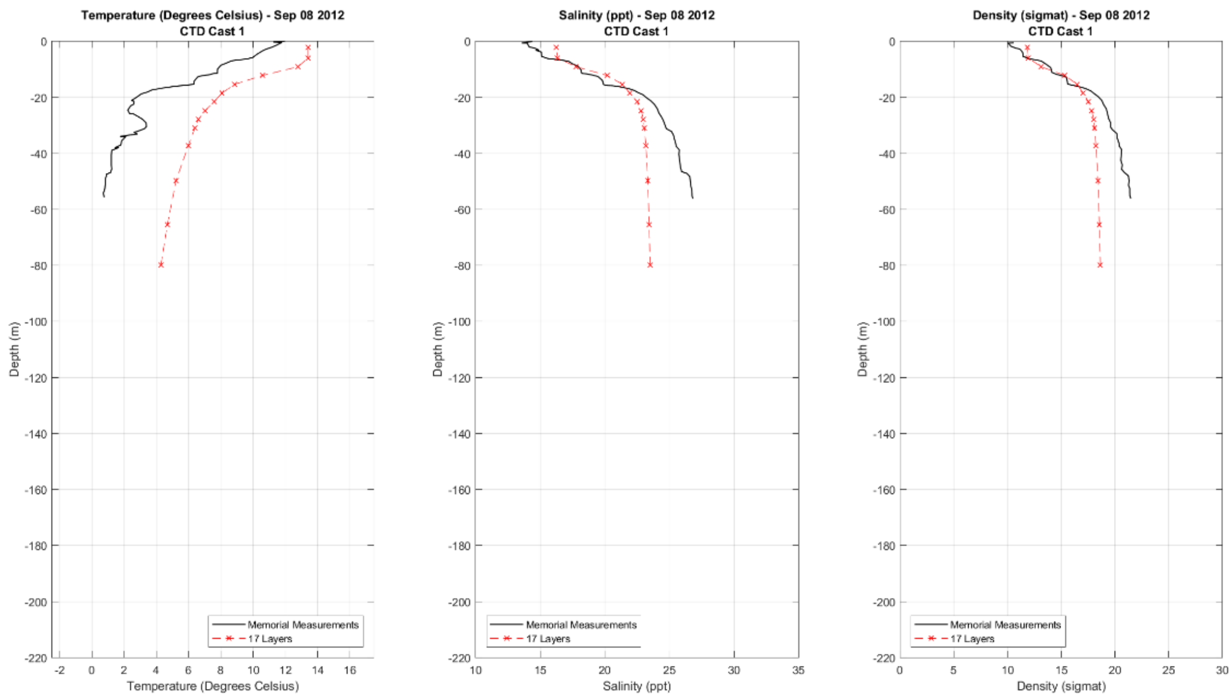

Figure 8 Comparison of measured-modelled temperature, salinity and density in east Lake Melville (CTD1)

Table 1 Model performance statistics for temperature, salinity and density (Means of each parameter)

Temperature (ºC)			
Bias	RMSE	Correlation	Skill
2.03	2.48	0.95	0.87

Salinity (ppt)			
Bias	RMSE	Correlation	Skill
2.29	2.60	0.96	0.85

Density (kg/m^3)			
Bias	RMSE	Correlation	Skill
1.67	1.92	0.96	0.89

Comparisons of measured and predicted mean velocity profiles are shown in Figure 9 and Figure 10 for Memorial ADCP locations M1 and M2, respectively. Overall, a reasonable agreement between the profiles is observed, although the deeper layers at site M2 show more bias towards tidal inflow at depth in the Narrows, which could be addressed with for more detailed offshore tide and current information but is not critical to support the conclusions of the analysis. Table 2 shows the summary statistics for velocity. Although the bias and RMSE values are low (which is desirable), correlation between measured and modelled velocities is lower than anticipated due to the lack of available local wind and tide data at the site. Model skill is fair for this parameter.

Table 2 Model performance statistics for flow velocity (Means of each parameter)

Velocity (m/s) u Direction			
Bias	RMSE	Correlation	Skill
-0.01	0.28	0.28	0.52

Velocity (m/s) v Direction			
Bias	RMSE	Correlation	Skill
0.00	0.16	0.19	0.46

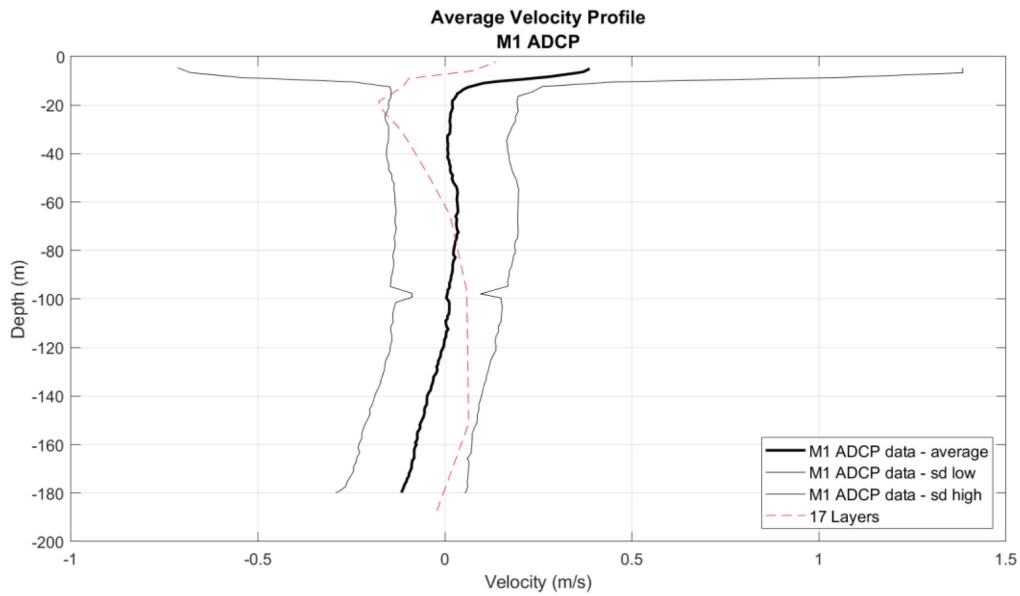

Figure 9 Comparison of measured and modelled mean velocity profiles at ADCP location M1. '17 Layers' = model predictions

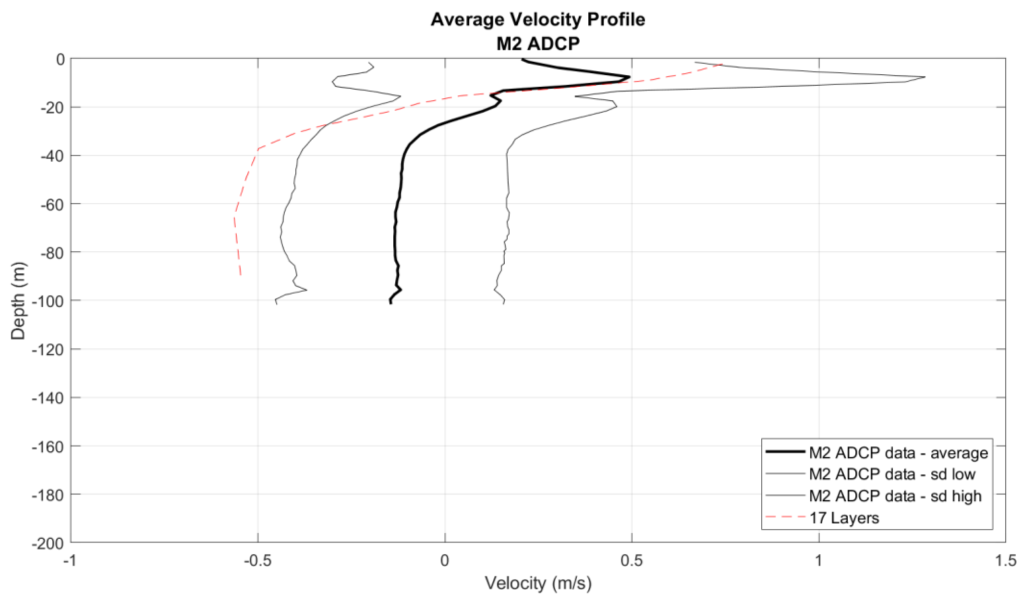

Figure 10 Comparison of measured and modelled mean velocity profiles at ADCP location M2. '17 Layers' = model predictions

Box Model Setup and Results

It was not possible to account for photodegradation and settling losses directly in the high resolution hydrodynamic model. Accordingly, a box model was set up to account for these losses. The box model used flow predictions from the hydrodynamic model to calculate the flux of water between Goose Bay, and the east and west parts of Lake Melville (Figure 11). The box model also considered the flux between vertical layers with depths of 0-3 m, 3-10 m, 10-20 m and >20 m. A schematic of the exchanges in the box model is shown in Figure 12.

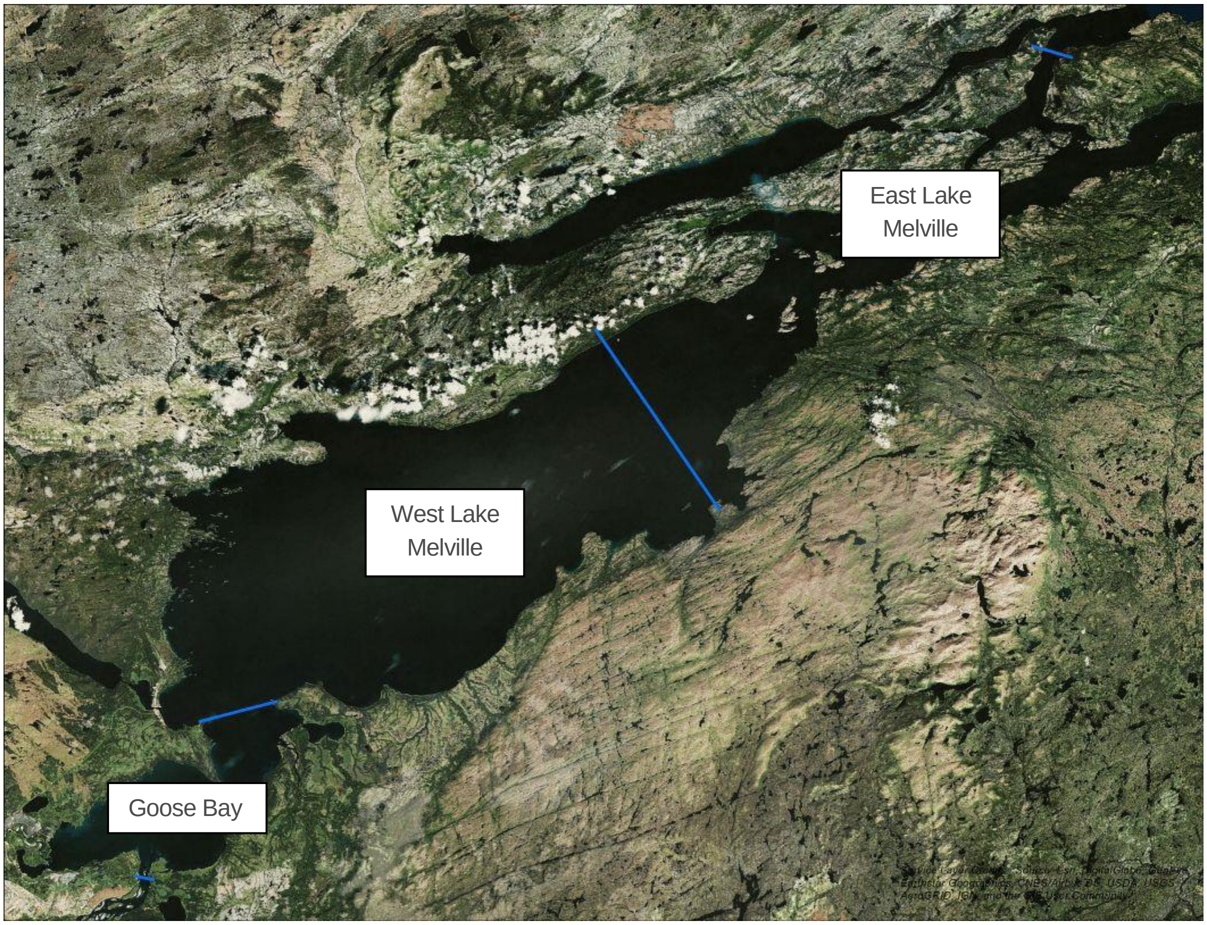

Figure 11 Areas considered in box model

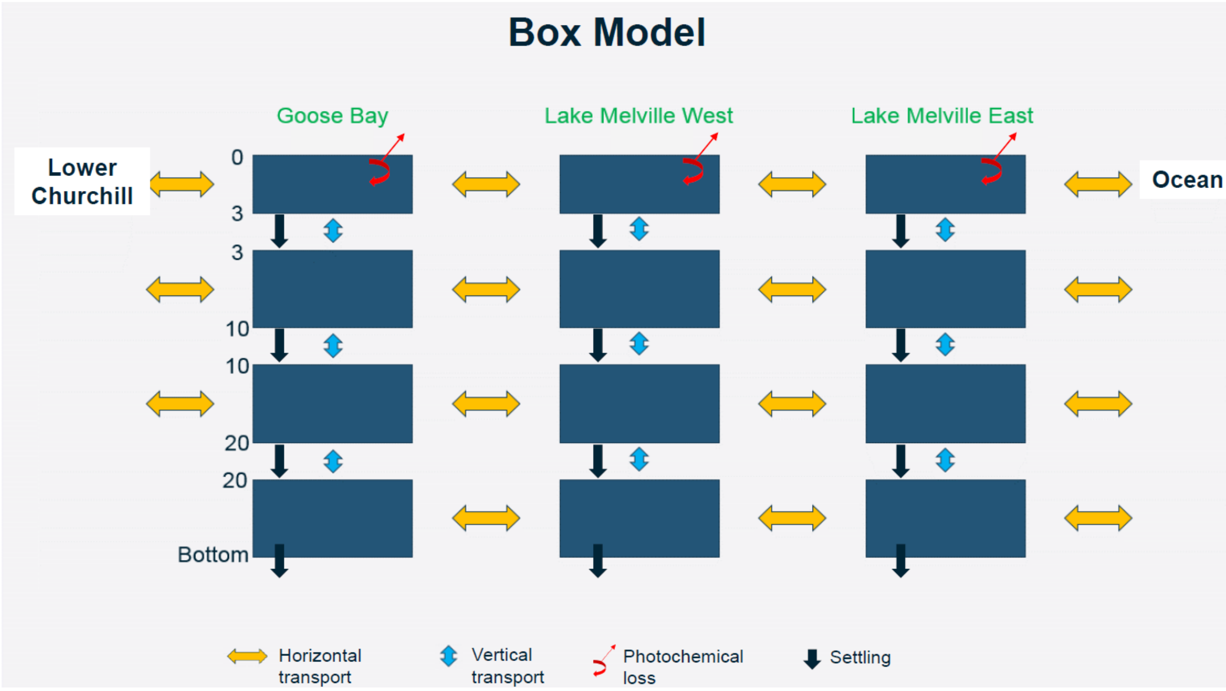

Figure 12 Schematic of box model configuration

Prior to simulating the effects of photodegradation and settling, the box model was calibrated with the goal of matching results of the simulation with the high-resolution model where MeHg was treated as a conservative (non-reactive) substance. Figure 13 shows the comparison of the two models for one of the twelve segments of the box model . Overall, the results in each segment of the box model matched well with the conservative simulation with the hydrodynamic model. The conservative models estimated a water residence time of approximately 11 days in Goose Bay and 125 days in Lake Melville.

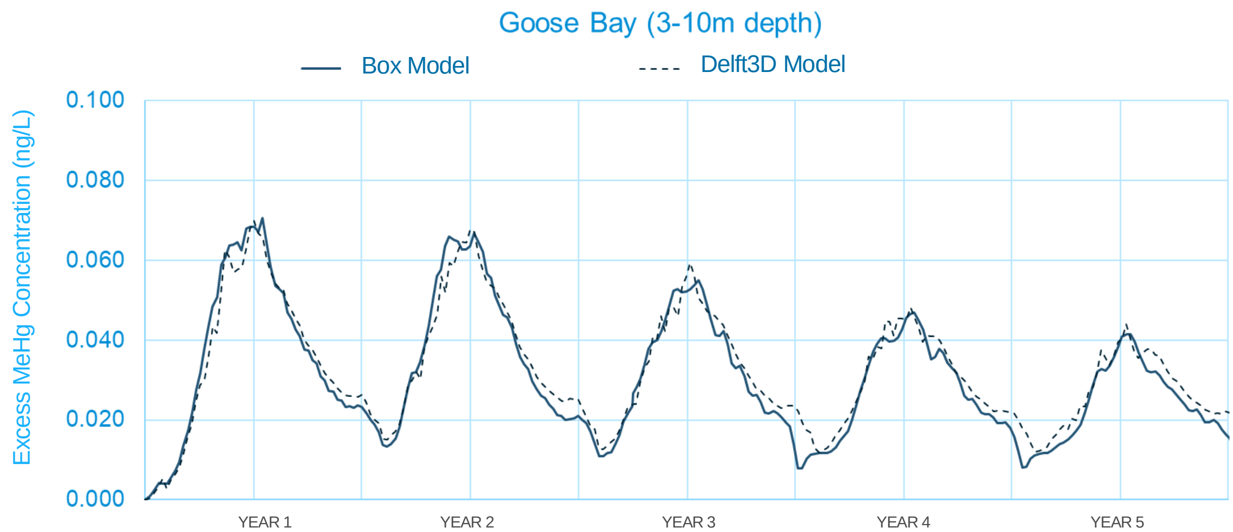

Figure 13 Comparison of Box Model and high resolution hydrodynamic model results for conservative simulation of excess MeHg in water.

Once the conservative mixing and dilution results from the high-resolution model were reasonably represented in the box model, losses due to photodegradation and settling were applied. Photodegradation rate constants (day^{-1}) were provided by Reed Harris using an analysis by Pollman (2018)[8] and were developed as follows:

- Photodegradation included components associated with UVA, UVB and PAR. Each component had a rate constant at the water surface, expressed as the inverse of incident radiation ($m^2\ E^{-1}$). When multiplied by incident radiation rates ($E\ m^{-2}\ day^{-1}$) the result had units of day^{-1}.
- This rate constants for each wavelength were multiplied by the dissolved MeHg concentration to estimate the rate of loss of MeHg in surface waters ($ng\ L^{-1}\ day^{-1}$). The dissolved concentration was assumed to be 70 percent of the unfiltered concentration, based on surface water sampling from 3 stations in Lake Melville from October 2016 – December 2017 .
- Photodegradation occurred during the ice free-season, assumed to occur for Julian days 152-305. Photodegradation was set to zero during the ice cover season.
- Radiation energy decreased with water depth. The extinction coefficients for UVA, UVB and PAR with depth resulted in 95% attenuation at a depth of 1 m for UVA, 0.5 m for UVB and ~3m for PAR.
- Two sets of photodegradation rate constants were used to bracket a range. The first set was based on Black et al (2012)[9] and the second set was based on Lehnherr and St. Louis (2009)[10].
- The average of model results for the two estimates of photodegradation losses was used in the final analysis.

[8] Pollman (2018) Unpublished review of methylmercury photodegradation in surface waters and approaches to modeling the reaction.
[9] Black, F.J., B.A. Poulin, and A.R. Flegal. 2012. Factors controlling the abiotic photo-degradation of monomethylmercury in surface waters. Geochim. Cosmochim. Acta 84: 492-507.
[10] Lehnherr, I. and V.L. St. Louis. 2009. Importance of ultraviolet radiation in the photodemethylation of methylmercury in freshwater ecosystems. Environ. Sci. Technol. 43: 5692-5698

Overall, the photodegradation loss estimate based on Black et al. (2012) ranged from 2-9 percent of the bulk phase per day, integrated over the top 3 m of the water column, during the ice-free season (average = 6.4% per day). The analogous range based on Lehnherr and St. Louis (2009) was approximately 0.5 to 3 percent per day in the ice-free season (average ~2% per day).

Figure 14 shows the effects of photodecomposition in one segment of the box model, using the rates developed using the Black et al. photodegradation constants. The dashed line shows results from the conservative simulation, and the solid line shows predicted concentrations after photodegradation losses. Photodegradation effects were more evident during the ice-free months, while levels returned towards the conservative condition during the months with ice cover as MeHg was replenished in the system. The response of lower depths in the lake was more muted as photodecomposition did not act directly on these layers, and the only effect on concentrations at depth was due to a reduced mass flux from the surface layer of the lake.

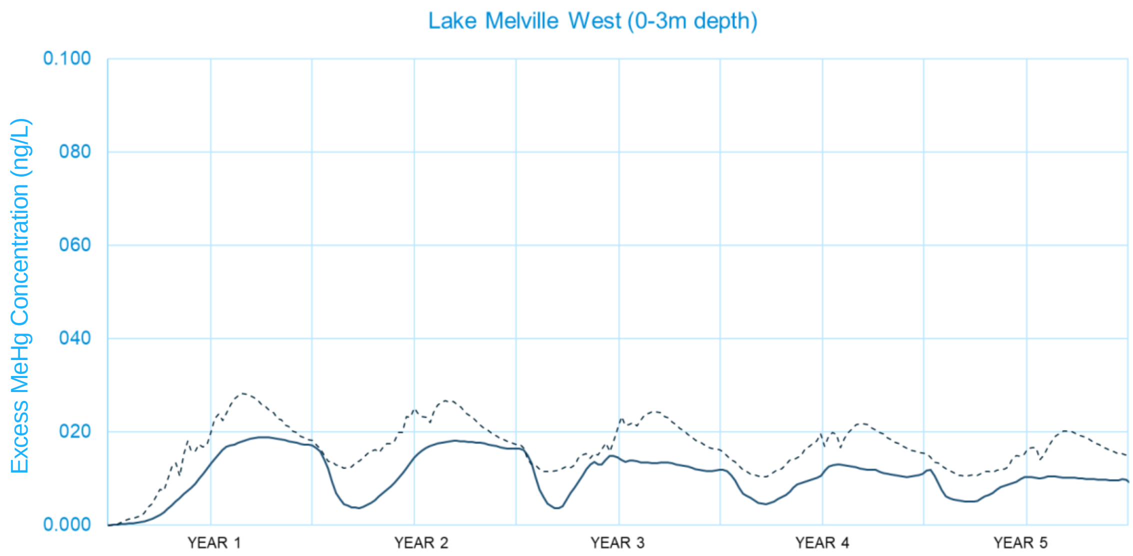

Figure 14 Effect of photodecomposition on predicted excess MeHg concentrations. Dashed line = conservative run; Solid line = with photodegradation. Results based on simulation using photodegradation constants from Black *et al*., (2012)

The effects of settling were also included in the box model. Based on the estimate that 70% of the unfiltered MeHg was dissolved, settling was applied to 30% of the water column MeHg mass in each segment of the box model. Three settling velocities (0.1 m/day, 0.5 m/day and 1.0 m/day) were tested in the box model. Each of these settling velocities is relatively conservative (meaning that higher MeHg concentrations will be predicted), representing the characteristics of the particulate organic carbon and fine clays upon which MeHg typically adsorbs more strongly. A full discussion of settling characteristics and the rationale for selection of settling velocity is beyond the scope of this memorandum, however the range of velocities used herein is considered conservative (i.e. it tends to under-estimate the amount of settling). A value of 0.5 m/day was used in the final analysis.

The effects of settling on predicted MeHg concentrations in surface waters are shown in Figure 15, for the box model compartment representing the top 3 m of Lake Melville West. The orange line shows the effects of settling and photodegradation. The fine dashed line shows photodegradation only, and the dashed line shows the conservative simulation.

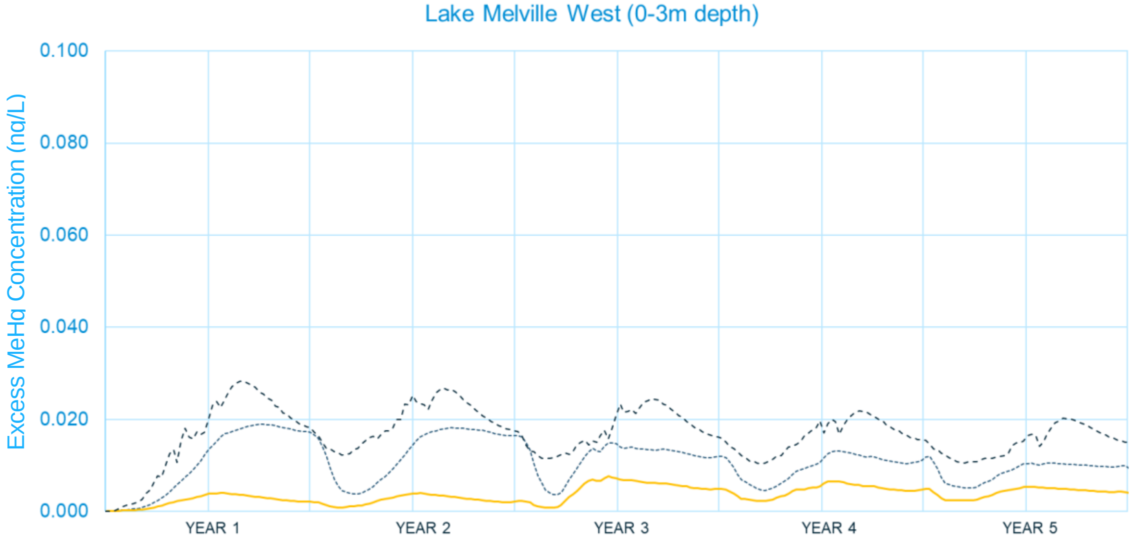

Figure 15 Effects of settling and photodegradation on excess MeHg concentrations in the box model, for the top 3 m of Lake Melville West. Upper dashed line = conservative run; fine dashed line = with photodegradation; orange line = with photodegradation and settling

The results from the overall model analysis are presented in Table 3 to Table 8. These tables summarise the results averaged for simulations using different loading scenarios (based on ResMerc and FLUDEX) and using the two estimates of photodegradation rate constants, along with a 0.5 m/day settling velocity for particulate MeHg. Excess concentrations in the top 20 m were 0.019 ng/L in Goose Bay (maximum 3-year average concentration), and 0.005-0.006 ng/L in Lake Melville (Table 3). Excess concentrations in the hypolimnion were lower, at 0.013 ng/L in Goose Bay, and 0.002-0.003 ng/L in Lake Melville (Table 4). Higher concentrations are to be expected in Goose Bay as it is a smaller waterbody, closer to the source in the lower Churchill River than Lake Melville. The increase in mass of MeHg in each area varied from 0.03-0.21 kg (Table 5 and Table 6). The relative increase over the baseline concentrations of MeHg estimated by Calder et al. (2016) was 1.9-2.1x in Goose Bay and 1.3 -1.4x in Lake Melville (Table 7 and Table 8). These values have been carried forward in the analysis by Wood (2018) to examine the relative degree of exposure by key species to elevated MeHg concentrations in Goose Bay and Lake Melville over time.

Table 3 Excess bulk MeHg water concentrations in the epilimnion (0-20 m)

Location	Excess MeHg Concentration: 3 Year average (ng/L, max)
Goose Bay	0.019
Melville West	0.006
Melville East	0.005

Table 4 Excess bulk MeHg water concentrations in the hypolimnion (Below 20 m)

Location	Excess MeHg Concentration 3 Year average (ng/L, max)
Goose Bay	0.013
Melville West	0.002
Melville East	0.003

Table 5 Increase in MeHg mass over baseline conditions in the epilimnion (0-20 m)

Location	Increase Over Baseline (Year 1-3 Average) (kg)
Goose Bay	0.06
Melville West	0.19
Melville East	0.06

Table 6 Increase in MeHg mass over baseline conditions in the hypolimnion (below 20 m)

Location	Increase Over Baseline (Year 1-3 Average) (kg)
Goose Bay	0.03
Melville West	0.21
Melville East	0.17

Table 7 Relative increase over baseline concentrations in the epilimnion (0-20 m). Baseline concentration: 0.017 ng/L for 0-20 m (from Calder et al., 2016).

Location	Peak/ Baseline
Goose Bay	2.1
Melville West	1.4
Melville East	1.3

Table 8 Relative increase over baseline concentrations (supplied by R. Baker) in the hypolimnion (below 20 m). Baseline concentrations below 20 m depth: 0.015 ng/L (Goose Bay), 0.007 ng/L (Lake Melville).

Location	Peak/Baseline
Goose Bay	1.9
Melville West	1.3
Melville East	1.4