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DATA DESCRIPTOR

Historical datasets (1950–2022) of monthly water balance components for the Laurentian Great Lakes

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This study develops a 73-year dataset of water balance components from 1950 to 2022 for the Laurentian Great Lakes Basins. This is carried out using the Large Lakes Statistical Water Balance Model (L2SWBM), which provides a Bayesian statistical framework that assimilates binational input datasets sourced from the United States and Canada. The L2SWBM infers feasible water balance component estimates through this Bayesian framework by constraining the output with a standard water balance equation. The result is value-added time series, including expressions of uncertainty, that ultimately close the water balance across the interconnected Great Lakes system. Therefore, the L2SWBM facilitates the understanding of discrepancies in datasets and hydroclimate parameters. This enhanced reliability stemming from coordinated data, with an understanding and quantification of uncertainty, could significantly boost confidence in decision support tools for water resources practitioners and policymakers. This joint effort advances scientific understanding and strengthens strategies and policies designed to bolster resilience in Great Lakes communities and its ecosystem in the face of a shifting climate.

Background & Summary

The Laurentian Great Lakes (Fig. 1), located in North America, are the largest freshwater system in the world, holding nearly 20% of the world's surface freshwater supply and home to over 30 million American and Canadian residents¹. The Great Lakes watershed supplies a regionally significant source of potable water and a complex ecosystem, encompassing a rich aquatic habitat, wetlands, woodlands, and densely urbanized areas. Additionally, the Great Lakes provide economic benefits to the region, which include recreation, shipping, and tourism. This highly populated region has been the focus of climate change studies in recent years, which provide insight into future lake levels and variability^{2–5}. An intensification of the hydrologic cycle, with more variable lake levels and longer periods of high and low water levels is expected as a result of a changing climate^{6–8}. This is evidenced by both record low water levels in some of the Great Lakes between 1998 and 2013⁹ and the recent record high water event throughout the Great Lakes between 2017 and 2020¹⁰, the latter of which resulted in pronounced socio-economic outcomes¹¹. The environmental, economic, and social factors described above underscore the importance of advancing hydrological modeling and data in the region.

Water balance components (i.e., over-lake evaporation, over-lake precipitation, and runoff) in watersheds with very large lakes can be challenging to estimate^{12,13}. Therefore, the large and varied geographic extent of the

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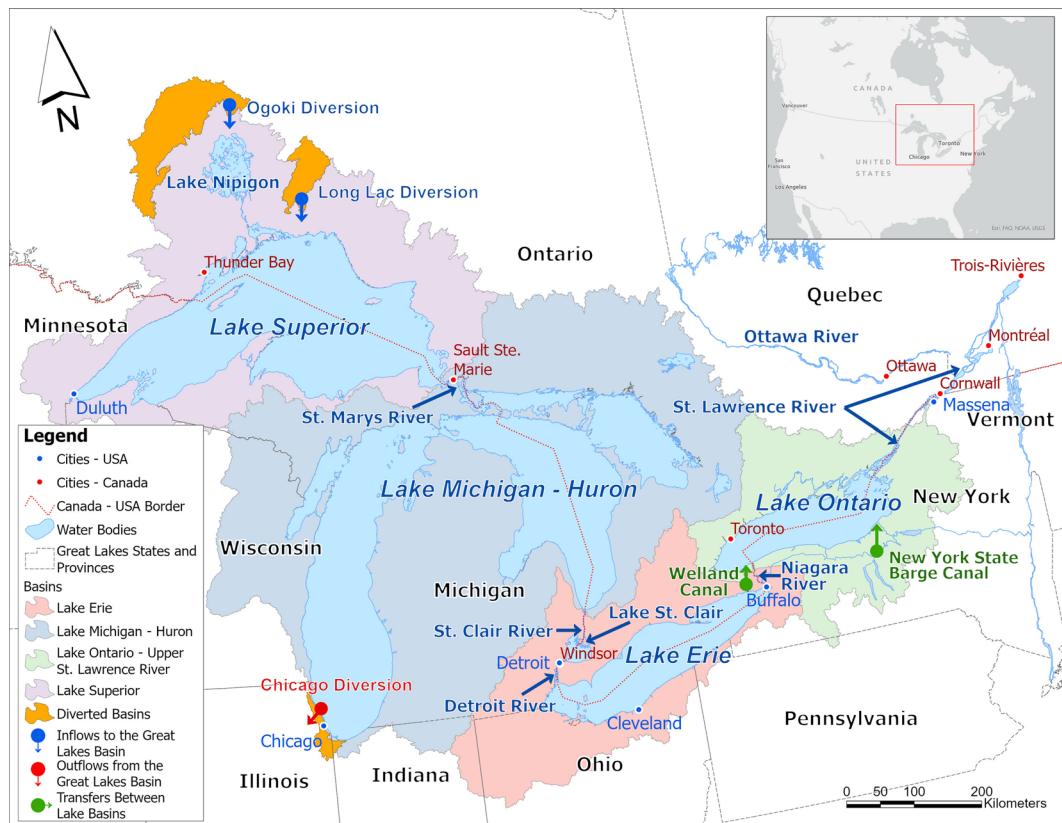


Fig. 1 Image of the Great Lakes subbasins, connecting channels, and diversions.

Data Source	Water Balance Component	Period of Record*	Used for Prior Distribution Estimation?	Used for Likelihood Function Estimation?	Data Reference
ECCC RDPA	P	2002–2022		Y	Fortin ¹⁶
CCGLHHD	H, I, Q, D, P	1900–2022	Y	Y	Gronewold <i>et al.</i> ¹⁴
NOAA-GELRL FVCOM	E	2018–2022		Y	Chen <i>et al.</i> ⁴² ; https://www.glerl.noaa.gov/res/glcfs/
NOAA-GLERL GLMHMD	R	2011–2022		Y	Hunter <i>et al.</i> ³⁴
GLSHyFS	P, E, R	1950–2022	Y	Y	Croley ³⁷ , Croley <i>et al.</i> ³⁸ ; Lofgren & Rouhana ⁴⁰ ; Hunter <i>et al.</i> ³⁴
IGS	I, Q	1900–2022		Y	Gronewold <i>et al.</i> ¹⁴
NOAA-NWS MPE	R	2008–2022		Y	Stevenson & Schumacher ¹⁷
ECCC NSRPS*	P, E, R	2022		Y	Fortin <i>et al.</i> ³⁶
NOAA NWM	R	1979–2020		Y	Johnson <i>et al.</i> ⁴¹
ECCC SWAT	R	2001–2022		Y	Shrestha <i>et al.</i> ⁵
ECCC WATFLOOD	R	2001–2022		Y	Shrestha <i>et al.</i> ⁵
ECCC WCPS	P, E, R	2016–2022		Y	Durnford <i>et al.</i> ³⁵
USACE Thiessen Polygons	P	2016–2022		Y	Hunter <i>et al.</i> ³⁴

Table 1. Overview of the datasets that were used as input into the L2SWBM, the associated water balance component data availability, the period of record of each input dataset, whether the data were used to estimate the prior distribution, if the data was used to estimate the likelihood function and an associated data reference for each water balance component. *Note that the period of record for NSRPS used for the final published datasets is up to the end of 2022; however, data extending to June 2023 were available and used for the correlation analysis, discussed in the following section.

Great Lakes watershed, the uniqueness of its large lakes, the complexity of simulating lake-atmosphere feedbacks, discontinuities of data at the international border¹⁴, and a comparatively sparse hydrometeorological gauging network provide challenges to physical models in accurately estimating water balance components. Additionally, hydrological model simulations suffer from data availability and data quality issues resulting in model validation and calibration challenges¹⁵. Precipitation data developed through gridded multisensory quantitative precipitation estimates, such as the Meteorological Service of Canada's Canadian Precipitation Analysis

Run ID	Model Run Details	Analysis Type
0	Operational model configuration	Status quo
1	ECCC WCPS precipitation removed	Leave-one-out
2	ECCC RDPA precipitation removed	Leave-one-out
3	NOAA-NWS MPE precipitation removed	Leave-one-out
4	CCGLHHD precipitation removed	Leave-one-out
5	USACE Thiessen polygons precipitation removed	Leave-one-out
6	GHSHyFS precipitation removed	Leave-one-out
7	ECCC NSRPS precipitation removed	Leave-one-out
8	ECCC WCPS evaporation removed	Leave-one-out
9	NOAA-GLERL FVCOM evaporation removed	Leave-one-out
10	GLSHyFS evaporation removed	Leave-one-out
11	ECCC NSRPS evaporation removed	Leave-one-out
12	NOAA-GLERL GLM-HMD runoff removed	Leave-one-out
13	ECCC WCPS runoff removed	Leave-one-out
14	ECCC WATFLOOD runoff removed	Leave-one-out
15	ECCC SWAT runoff removed	Leave-one-out
16	GLSHyFS runoff removed	Leave-one-out
17	ECCC NSRPS runoff removed	Leave-one-out
18	NOAA NWM runoff removed	Leave-one-out
19	All ECCC WCPS water balance components removed	Leave-one-out
20	All GLSHyFS water balance components removed	Leave-one-out
21	All ECCC NSRPS water balance components removed	Leave-one-out
22	No Welland Canal discharge	Diversion sensitivity
23	No Chicago Diversion discharge	Diversion sensitivity
24	No Long Lac Diversion discharge	Diversion sensitivity
25	No Ogoki Diversion discharge	Diversion sensitivity
26	No diversion discharge	Diversion sensitivity
27	No historical coordinated precipitation, only ECCC WCPS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
28	No historical coordinated precipitation, only ECCC WCPS evaporation, and no ECCC SWAT runoff	Least Correlated
29	No ECCC NSRPS precipitation, only WCPS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
30	No ECCC NSRPS precipitation, only ECCC WCPS evaporation, and no ECCC SWAT runoff	Least Correlated

Table 2. Summary of experimental runs, including the Run IDs 0 to 30, model run details, and analysis type.

(CaPA)¹⁶, the National Weather Service Multisensor Precipitation Estimator (MPE)^{17,18]}, and the National Severe Storm Laboratory's Multi-Radar/Multi-Sensor (MRMS)¹⁹ have resulted in advancements in the resolution of the Great Lakes water balance, however, estimating all water balance components remains challenging.

The goal of this article is to present updated water balance component datasets of the Laurentian Great Lakes over-lake precipitation, over-lake evaporation, and lateral tributary inflow for a seventy-three year period from 1950 to 2022 using the Large Lakes Statistical Water Balance Model, henceforth referred to as the L2SWBM^{20,21}. The L2SWBM provides a Bayesian statistical framework for the assimilation of independent datasets and calculates water balance components by constraining estimates with a conventional water balance equation. This results in water balance component estimates that close the water balance over several time periods. The L2SWBM is used operationally, on a monthly basis, in support of the Coordinating Committee on Great Lakes Hydraulic and Hydrologic Data (CCGLHHD) (henceforth known as the Coordinating Committee) (<https://www.greatlakescc.org/en/home/>). Additionally, work is underway to use the L2SWBM to coordinate net basin supply (NBS) components on a monthly basis. The Coordinating Committee is an ad hoc committee comprised of experts from government organizations from the United States (US) and Canada, who are responsible for the collection, coordination and dissemination of the hydraulic, hydrologic, and vertical control data required for water management and research purposes in the Great Lakes and St. Lawrence River. The L2SWBM output is also used in support of the International Joint Commission's (IJC) International Lake Ontario – St. Lawrence River Board and the IJC Great Lakes Adaptive Management (GLAM) Committee. Significant effort and collaboration have resulted in binationally coordinated data products and marked advancements in monitoring and modeling of Great Lakes hydraulic and hydrologic conditions²². However, continued binational collaborative research is needed to continue to advance this work²³.

This manuscript builds upon the work of Do *et al.*²⁴ who presented a seventy-year record of Lake Superior, Lake Michigan-Huron, Lake Erie, and Lake Ontario water balance components using the L2SWBM. The current operational L2SWBM includes several additional input datasets that were not included in the Do *et al.*²⁴ simulation, incorporates data updates and bug fixes that result in improved connecting channel flow estimates, and extends the period of record to 2022. The present research additionally focuses on the performance of the L2SWBM when run with different subsets of input data to determine an optimal configuration. Furthermore,

Run ID	Model Run Details	Analysis Type
31	No historical coordinated precipitation, only NOAA-GLERL FVCOM evaporation, and no ECCC WATFLOOD runoff	Least Correlated
32	No historical coordinated precipitation, only NOAA-GLERL FVCOM evaporation, and no ECCC SWAT runoff	Least Correlated
33	No NSRPS precipitation, only NOAA-GLERL FVCOM evaporation, and no ECCC WATFLOOD runoff	Least Correlated
34	No ECCC NSRPS precipitation, only NOAA-GLERL FVCOM evaporation, and no ECCC SWAT runoff	Least Correlated
35	No historical coordinated precipitation, only ECCC NSRPS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
36	No CCGLHHD precipitation, only ECCC NSRPS evaporation, and no ECCC SWAT runoff	Least Correlated
37	No ECCC NSRPS precipitation, only ECCC NSRPS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
38	No ECCC NSRPS precipitation, only ECCC NSRPS evaporation, and no ECCC SWAT runoff	Least Correlated
39	No CCGLHHD precipitation, only GLSHyFS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
40	No CCGLHHD precipitation, only GLSHyFS evaporation, and no ECCC SWAT runoff	Least Correlated
41	No ECCC NSRPS precipitation, only GLSHyFS evaporation, and no ECCC WATFLOOD runoff	Least Correlated
42	No ECCC NSRPS precipitation, only GLSHyFS evaporation, and no ECCC SWAT runoff	Least Correlated
43	GLSHyFS, NOAA-WMS MPE, and ECCC RDPA precipitation, GLSHyFS, NOAA-GLERL FVCOM, and ECCC WCPS evaporation, and ECCC SWAT, ECCC WCPS, GLSHyFS, and ECCC WATFLOOD runoff	Best Model Skill
44	5 additional randomly selected and permuted evaporation datasets, 4 runoff, and 5 precipitation	Permuted and Infilled
45	ECCC RDPA precipitation prior, GLSHyFS evaporation prior, and ECCC SWAT later tributary inflow prior	Prior sensitivity
46	Model run with ECCC RDPA precipitation, NOAA-GLERL FVCOM evaporation, and ECCC WATFLOOD runoff	Limited input data

Table 3. Summary of experimental runs, including the Run IDs 31 to 46, model run details, and analysis type.

	ECCC WCPS	ECCC RDPA	NOAA-NWS MPE	CCGLHHD	USACE Thiessen Polygons	GLSHyFS
ECCC WCPS	1	0.815	0.913	0.919	0.872	0.925
ECCC RDPA	0.815	1	0.825	0.797	0.729	0.832
NOAA-NWS MPE	0.913	0.825	1	0.938	0.892	0.943
CCGLHHD	0.919	0.797	0.938	1	0.976	0.991
USACE Thiessen Polygons	0.872	0.729	0.892	0.976	1	0.956
GLSHyFS	0.925	0.832	0.943	0.991	0.956	1

Table 4. Cross-correlation matrix of Lake Michigan-Huron over-lake precipitation from November 2016 to December 2020.

	ECCC WCPS	NOAA-GLERL FVCOM	GLSHyFS
ECCC WCPS	1	0.960	0.957
NOAA-GLERL FVCOM	0.960	1	0.962
GLSHyFS	0.957	0.962	1

Table 5. Cross-correlation matrix of Lake Michigan-Huron over-lake evaporation from January 2018 to December 2022.

measures of model skill, uncertainty, and model closure are used to assess model performance. Ultimately, data-sets of basin-wide average precipitation, runoff, and evaporation for each of the Laurentian Great Lakes are estimated. This data is intended for use by hydrologists, engineers, decision-makers, and other users for research and water management purposes throughout the Great Lakes Basin.

Large lakes statistical water balance model (L2SWBM). The modeling framework of the L2SWBM implements a water balance model by constraining water balance components over monthly, yearly, and 5-year time periods. The water balance for lakes Superior, Michigan-Huron, Erie and Ontario can be defined through the change in storage over a given time period, as provided in Eq. (1)²⁰.

$$\Delta H_{j,w} = H_{j+w} - H_j = \sum_{i=j}^{j+w-1} (P_i - E_i + R_i + I_i - Q_i \pm D_i + \epsilon_i) \quad (1)$$

Where $\Delta H_{j,w}$ is the change in lake storage over w months, starting with month j , H_j is the water level at the beginning of month j , H_{j+w} is the water level at month $j + w$, P_i is the over-lake precipitation (mm), E_i is the over-lake evaporation (mm), R_i is lateral tributary inflow (or runoff) (mm), I_i is inflow from upstream lakes (mm normalized over lake area), Q_i is the outflow to downstream lakes (mm normalized over lake area), D_i is the inter-basin diversions (mm normalized over lake area), and ϵ_i is a process error term intended to account for sources of water balance uncertainty that are not accounted for by the other water balance components such as thermal expansion, glacial isostatic rebound, and groundwater fluxes^{25,26}. Note that the sign of D_i is dependent on diversion direction (either in or out of a given lake). Also, a rolling window of 12 months (w) is used herein,

	NOAA-GLERL GLM-HMD	ECCC WATFLOOD	ECCC SWAT	GLSHyFS	NOAA NWA
NOAA-GLERL GLM-HMD	1	0.901	0.894	0.940	0.886
ECCC WATFLOOD	0.901	1	0.957	0.902	0.896
ECCC SWAT	0.894	0.957	1	0.906	0.878
GLSHyFS	0.940	0.902	0.906	1	0.908
NOAA NWA	0.886	0.896	0.878	0.908	1

Table 6. Cross-correlation matrix of Lake Michigan-Huron runoff from January 2001 to March 2016.

as it typically provides improved water balance closure^{20,21}. The comparatively small lake-surface area of Lake St. Clair results in its water balance being dominated by inflows from the St. Clair River and outflows from the Detroit River. It is accordingly run in a different configuration in the L2SWBM model, but since its water balance components are not the focus of this analysis, it will not be discussed further herein. Probabilistic water balance component estimates are inferred through a Bayesian approach, where prior distributions and likelihood functions are parameterized from specified independent data sources and expert knowledge and opinion. Water balance components developed through the model are considered the “true” estimates, given they are appropriately constrained by the closure of the water balance.

The likelihood function for the change in storage within a given lake over a period of w months is given by²⁰:

$$y_{\Delta H_j, w} = y_{H_{j+w}} - y_{H_j} \sim N(\Delta H_{j, w}, \tau_{\Delta H_{j, w}}) \quad (2)$$

where $y_{\Delta H_j, w}$ is the observed change in storage, starting in month j and over the rolling window of length w , $y_{H_{j+w}}$ is the water level measurements at the beginning of month $j + w$, y_{H_j} is the water level measurements at the beginning of month j , the difference of which is modeled with a normal distribution with mean $\Delta H_{j, w}$ and precision $\tau_{\Delta H_{j, w}}$. In this formulation of the L2SWBM, the normal distribution is parameterized using the precision, rather than the variance, following Bayesian inference convention^{27–29}. The precision of the data sources of each water balance component at each time step were modeled with a noninformative gamma prior probability distribution with both shape and scale parameters equal to 0.1^{28,30}. The bias of channel flow; however, was modeled using a normal distribution with mean 0 and precision of 0.01³¹.

Priors are modeled with normal probability distributions for over-lake evaporation (E_m), inflow (I_m), outflow (Q_m), and diversions (D_m), where m is the calendar month. These water balance components were modeled using empirical estimates of input data spanning from 1950 to 2022, which is discussed further below and presented in Table 1. For example, the prior probability distribution of inflow (connecting channel flow) is modeled as follows:

$$\pi(I_m) = N(\mu_{I_m}, \tau_{I_m}) \quad (3)$$

where $\pi(I_m)$ is the prior probability distribution of inflow, μ_{I_m} is the mean and τ_{I_m} is the precision. Q_m , D_m , and E_m are similarly modeled, however the precision of over-lake evaporation is divided by two (variance is doubled) to account for the strong historical seasonality and low variability in this water balance parameter. The prior for over-lake precipitation (P_m) is modeled using a gamma probability distribution and the prior for runoff (R_m) with a lognormal probability distribution, with the parameters of each distribution being estimated empirically through historical data. Finally, the error term (ϵ_i) is modeled using a vague prior distribution. For a more detailed description of the probability distribution used herein, please refer to Do *et al.*²⁴ or Gronewold *et al.*²⁰.

The L2SWBM infers water balance component estimates from the posterior distribution for a period ranging from 1950 to 2022 and is coded in the R programming language³². Parameter estimates for the likelihood and prior probability distributions, are encoded via Just Another Gibbs Sampler (JAGS) but more specifically the ‘rjags’ package³³. For the published dataset, the JAGS model was simulated over 1,000,000 Markov Chain Monte Carlo (MCMC) iterations using three parallel MCMC chains. The model evaluation runs were similarly carried out; however, due to their computational expense, were run using the Coordinating Committee’s operational configuration of the most recent 10 years (2013 to 2022) and with 200,000 MCMC iterations. In both instances, the first half of the iterations are considered the “burn-in” period and discarded. The remaining data is subsequently thinned, resulting in a final dataset of 2000 iterations. The data are additionally used to infer feasible parameter ranges of the 95% credibility interval. In keeping with best practice, no observations were used to estimate both the prior distribution and likelihood functions, therefore, the 1,000,000 trial model was run in two parts, the first spanning from 1950 to 1987 and the second from 1988 to 2022. The priors for the 10-year operational model were selected from data ranging from 1950 to 2012.

Independent data sources used in the L2SWBM. The focus of this manuscript is on the optimization of precipitation, evaporation, and runoff water balance components. Independent data sources that are operational products used by federal agencies on both sides of the border for tracking Great Lakes water budget changes were selected for this research. The data sources used as input to the L2SWBM for this work include:

- Over-lake precipitation: 7 independent datasets are included in the L2SWBM model, which include (1) the National Oceanic and Atmospheric Administration’s (NOAA) National Weather Service (NWS) Multisensor Precipitation Estimator (MPE)^{17,18}, (2) Environment and Climate Change Canada’s (ECCC) Regional

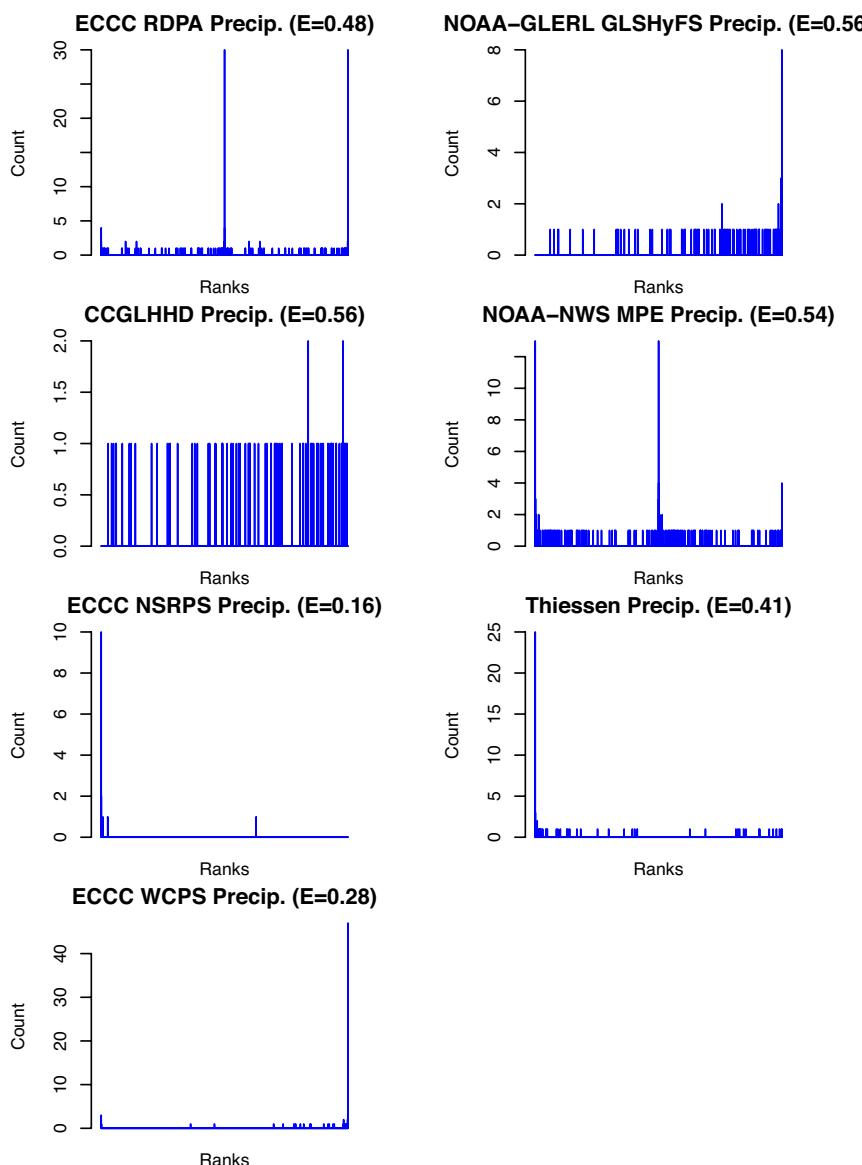


Fig. 2 Rank histograms of the independent datasets of over-lake precipitation from the operational model (Run ID 0) of over-lake precipitation for Lake Superior. Note: E denotes entropy.

Deterministic Precipitation Analysis (RDPA)¹⁶, (3) historical coordinated precipitation from the Great Lakes Coordinating Committee (CCGLHHD, found at <https://doi.org/10.5281/zenodo.10479324>), (4) United States Army Corps of Engineers (USACE) interpolated Thiessen Polygons³⁴, (5) historical precipitation from Environment and Climate Change Canada's Water Cycle Prediction System (WCPS) analysis³⁵, (6) precipitation from the Great Lakes Seasonal Hydrological Forecasting System (GLSHyFS)³⁴, and (7) Environment and Climate Change Canada's National Surface and River Predicting System (NSRPS)³⁶.

- Over-lake evaporation: there are 4 independent datasets of evaporation in the L2SWBM model, which include (1) historical over-lake evaporation from the WCPS analysis³⁵, (2) the Finite-Volume Primitive Equation Community Ocean Model (FVCOM, described by Chen *et al.*³⁷), as run in NOAA-GLERL's experimental Great Lakes Coastal Forecast System (<https://www.glerl.noaa.gov/res/glcfs/>), (3) over-lake evaporation from GLSHyFS³⁸, and (4) over-lake evaporation from NSRPS³⁶.
- Lateral tributary inflow: 7 sources of independent runoff are included in the L2SWBM (1) lateral tributary inflow from the NOAA-GLERL Great Lakes Monthly Hydrometeorological Database (GLM-HMD)³⁴, (2) historical runoff from the WCPS analysis³⁵, (3) WATFLOOD⁵, (4) Soil & Water Assessment Tool (SWAT)⁵, (5) runoff from GLSHyFS^{39,40}, and (6) NOAA's National Water Model (NWM)⁴¹.

Other sources of data are included in the model and are summarized in Table 1, in addition to the aforementioned data sources. As indicated in the table, data provided by the Coordinating Committee were used as priors to the model for lake storage, connecting channel flow and diversion flow. Data from GLSHyFS were used to estimate the prior distribution for precipitation, evaporation, and runoff as it has a long period of available

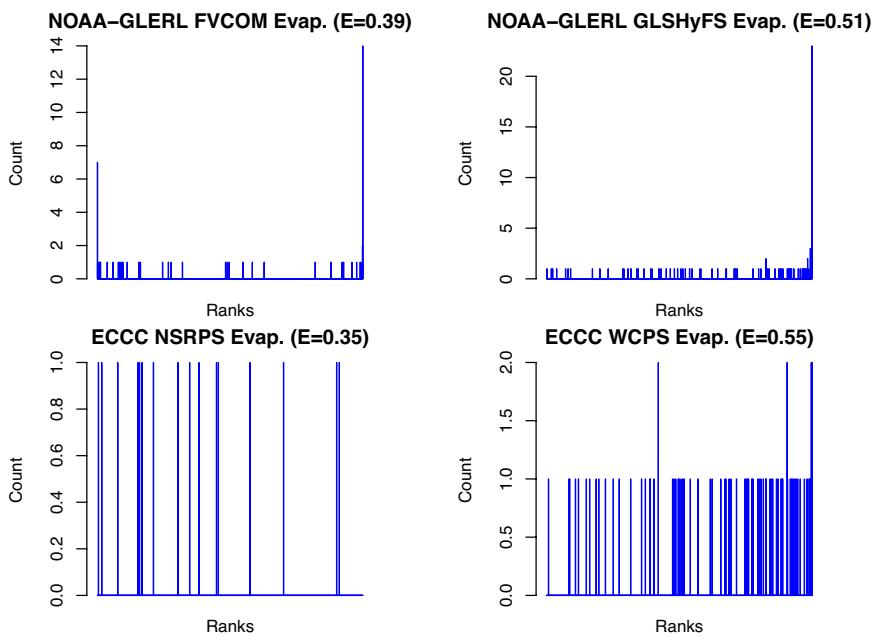


Fig. 3 Rank histograms of the independent datasets of over-lake evaporation from the operational model (Run ID 0) of over-lake evaporation for Lake Superior. Note: E denotes entropy.

record. Several additional datasets were added to the operational version of the L2SWBM since the Do *et al.*²⁴ publication. The following section will provide an overview of experimental runs conducted to determine if there is value in the addition of new datasets to the model or if an optimal subset of data can improve model performance and subsequent output.

Methods

For the current analysis, a series of experiments was carried out to determine if an optimal selection of input data could be used to improve model output. To this end, model performance was evaluated by the model's ability to close the water balance, reductions in uncertainty, and the reliability of the ensemble (or model skill) through rank histograms. The L2SWBM attempts to close the water balance over a rolling window of 60 months (5-year), 12 months (1-year), and monthly. Through this study, it was determined that the model is capable of adequately closing the 1-year and 5-year water balances, therefore, the focus herein is on improvements in monthly water balance closure. Furthermore, monthly data is important for regulation and water management purposes and forecasting in the Great Lakes basins. The model closure calculation is obtained by first estimating model outputs of simulated detention storage for each month it is run (i.e. 73 years or 876 months). Empirical 95% confidence intervals are then calculated using the ensemble data for each month. If the actual (measured) detention storage falls within the 95% confidence interval of the empirical quantile, that monthly water balance is considered closed. Model closure is summarized as follows:

$$C = \frac{N_c}{N_T} \quad (4)$$

where C is the reported L2SWBM monthly closure, N_c is the number of months the model closes the water balance as previously described, and N_T is the total number of months the model is run. Reduction in uncertainty is measured by the average difference in the upper (97.5%) and lower (2.5%) reported credible intervals for water balance components, where a decrease in uncertainty is considered an improved result.

Model skill is assessed with a measure of improvement in rank histograms of model output against three selected datasets that are generally considered to be best estimates based on expert opinion, namely residual net basin supply (NBS_r), which is available from the CCGLHHD, ECCC RDPA precipitation, and NOAA-NWS MPE precipitation. NBS_r is derived from the water balance provided in Eq. 1, however, the equation is rearranged into NBS_r and component net basin supply (NBS_c), which is given by:

$$\Delta H - I + Q \pm D = P + R - E + \epsilon \quad (5)$$

Or:

$$NBS_r = NBS_c + \epsilon \quad (6)$$

Given that the change in lake storage (ΔH), connection channel flow (I and Q), and diversion flow (D) are measured with a high degree of accuracy and internationally coordinated, NBS_r is considered precise and an optimal dataset for which to compare model output. Monthly NBS_r data is available from the CCGLHHD

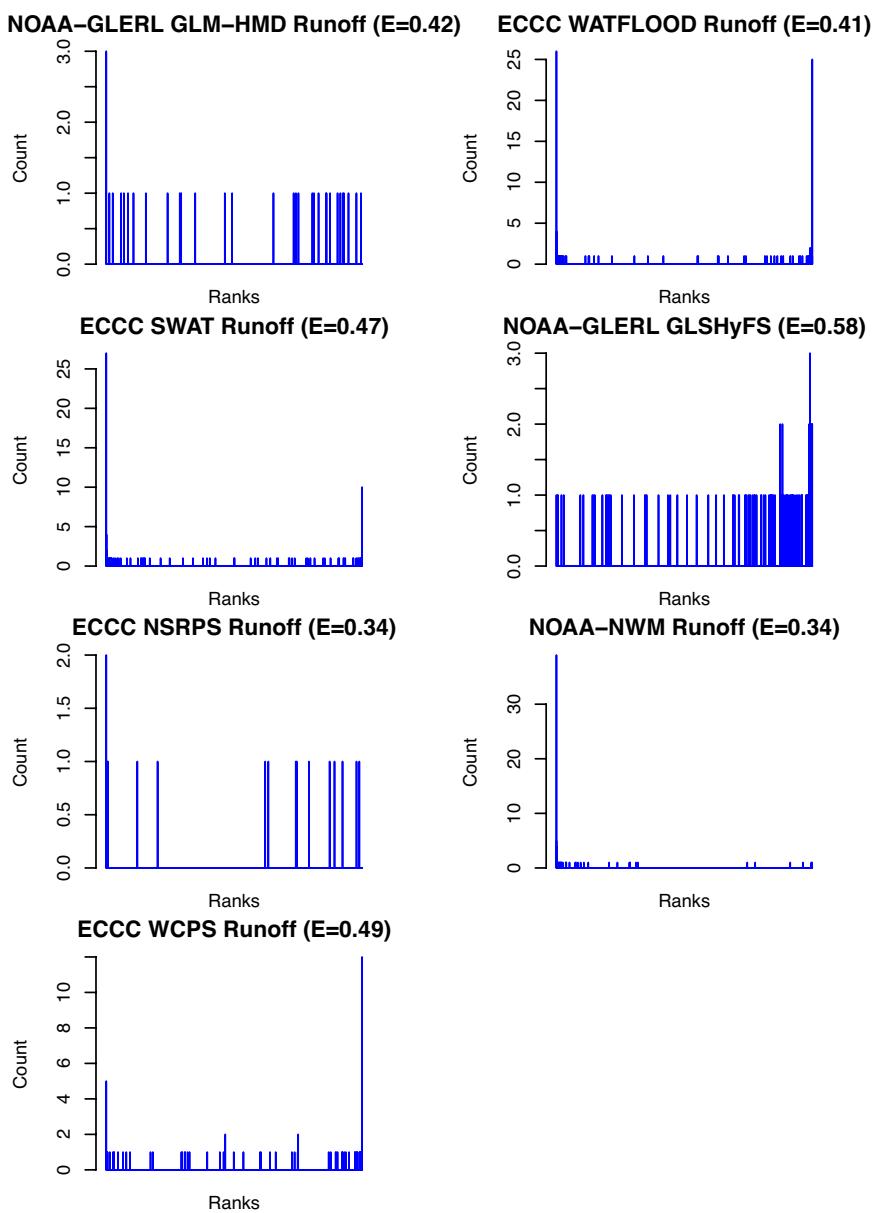


Fig. 4 Rank histograms of the independent datasets of lateral tributary inflow from the operational model (Run ID 0) of lateral tributary inflow for Lake Superior. Note: E denotes entropy.

website. Additionally, Lespinas *et al.*¹⁵ and Kiltzmillier *et al.*¹⁸ highlight the accuracy of the ECCC RDPA and MPE, respectively. The flatness of the rank histograms is measured using an entropy statistic^{43,44}. Entropy is a flatness measure ranging from 0 to 1, with zero representing a rank histogram with all counts in a single bin and 1 being perfectly flat.

Experimental design. A number of experiments are carried out to determine if an optimal configuration of input data can improve L2SWBM output results. These included a series of leave-one-out runs, sensitivity to diversion flows, a series of runs with subsets of least correlated data, running the model with only those datasets having the best model skill, running the operational model with updated prior beliefs, and a model run with additional permuted datasets. An overview of these model runs is provided in Tables 2 and 3.

The initial run (Run ID 0) is the status quo model and serves as a basis of comparison for the remaining experimental runs. Run IDs 1–21 are leave-one-out experiments where datasets are sequentially removed from the model runs. Of note, Run IDs 19, 20, and 21 omit the full model datasets (i.e. precipitation, evaporation, and runoff) for the ECCC WCPS, GLSHyFS, and ECCC NSRPS models, respectively. In Run IDs 22 to 26, diversion discharge is sequentially removed from the model runs to ascertain the model's sensitivity to each of the Great Lakes diversions. Run IDs 27 to 42 were developed by assessing cross-correlation between datasets. It is important to provide the L2SWBM with independent datasets, given that highly correlated data may skew the output in their favour. Using Lake Michigan-Huron as an example, the Pearson correlation matrices of the overlapping

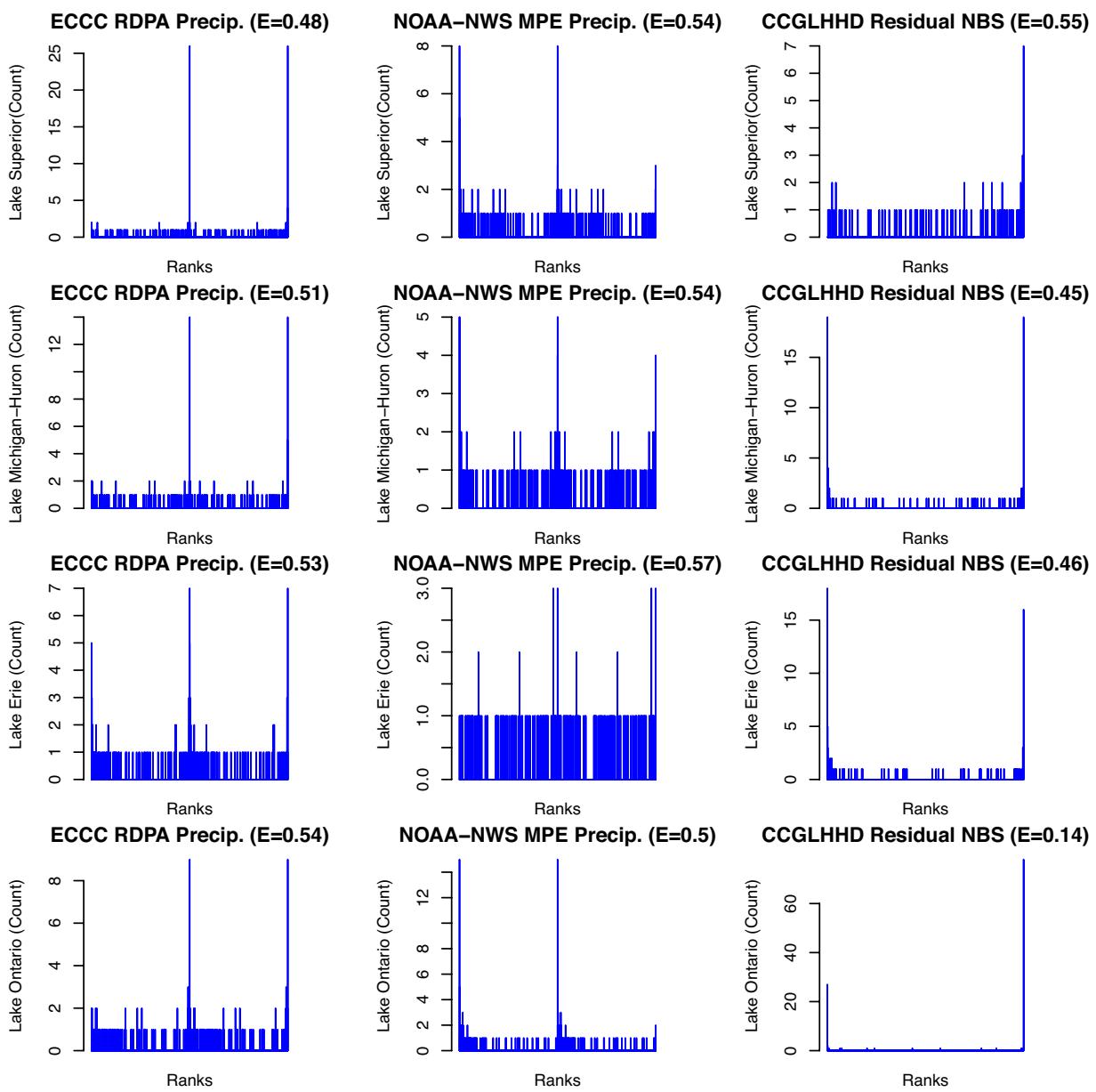


Fig. 5 Rank histograms of L2SWBM over-lake precipitation model output and RDPA, NOAA-NMS MPE, and L2SWBM NBS_c and CCGLHHD NBS_r for Lake Superior, Lake Michigan-Huron, Lake Erie, and Lake Ontario for Run ID 4. Note: E denotes entropy.

periods of record for the precipitation, evaporation, and runoff datasets are provided in Tables 4–6. Please refer to the Supplementary Information for the complete correlation analysis for lakes Superior, Michigan-Huron, Erie, and Ontario. Table 4 indicates that correlation among precipitation datasets is high, however, this is expected with measures of the same water balance component. Of note, is the relationship between the GLSHyFS dataset and the historical coordinated precipitation data (CCGLHHD). These consistently high correlations between datasets are a result of the CCGLHHD precipitation dataset using GLSHyFS for its precipitation data, beginning in 1948. A similar analysis was carried out for lakes Superior, Erie, and Ontario, which provided similar results that are presented in Tables S1–S21. For this reason, the historical coordinated precipitation is removed from the L2SWBM as it was not sufficiently independent. Also of note, correlations were calculated for overlapping periods of record only, therefore, certain datasets are not included in Tables 4–6 but are available in the Supplementary Information. Thirteen model runs (Run ID 27 to 42) were selected to determine if model output improvements could be realized when the L2SWBM was run with a subset of least correlated data.

The input datasets for Run ID 43 are selected based on the model skill of the operational version of the model. Model skill is evaluated through the examination of rank histograms of the water balance components of over-lake precipitation, over-lake evaporation, and lateral tributary inflow. Figure 2 shows the seven independent datasets included in the L2SWBM for Lake Superior for over-lake precipitation. For the sake of brevity, rank histograms of the remaining lakes are provided in Figures S1–S9. The historical coordinated (CCGLHHD)

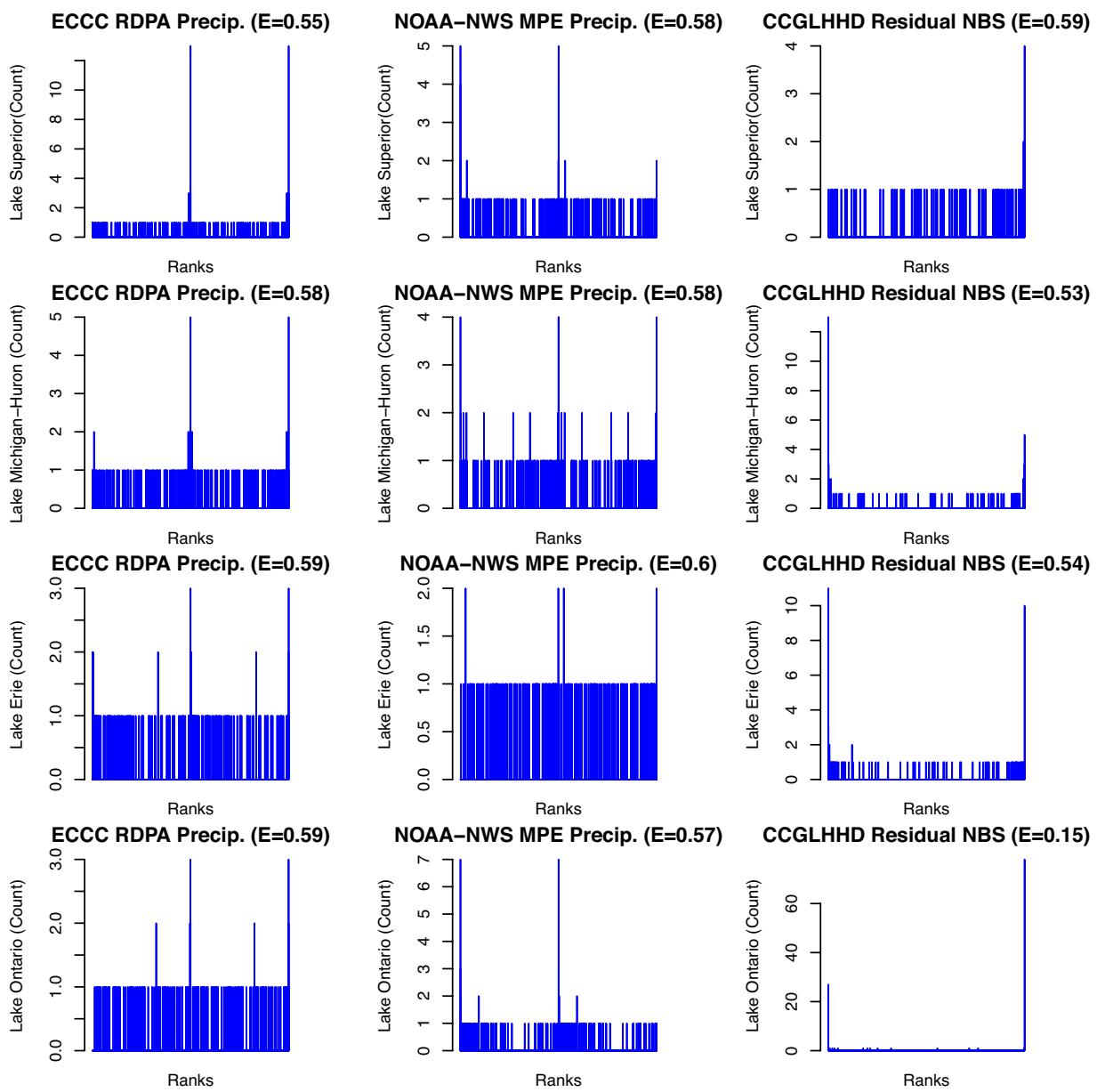


Fig. 6 Rank histograms of L2SWBM over-lake precipitation model output and RDPA, NOAA-NMS MPE, and L2SWBM NBS_c and CCGLHHD NBS_r for Lake Superior, Lake Michigan-Huron, Lake Erie, and Lake Ontario for Run ID 43. Note: E denotes entropy.

rank histogram appears to be the most balanced with others showing positive or negative bias. Based on the magnitude of the entropy elucidated in Fig. 2 and Figs. S1–S3 and denoted by E, where 0.5 is selected as the cutoff, ECCC RDPA, NOAA-GLERL GLSHyFS, CCGLHHD, and NOAA-NWS MPE over-lake precipitation provide the best model skill. The skill of over-lake evaporation is provided in Fig. 3 and Figs. S4–S6, where ECCC WCPS, NOAA-GLERL GLSHyFS, and NOAA-GLERL FVCOM have the best result. The rank histogram of NOAA-GLERL FVCOM indicates some potential for lack of variability for Lake Superior but does provide stronger results in other lakes (provided in the Supplementary Information). Finally, Figs. 4, S7–S9 provide the model skill for lateral tributary inflow, where overall, ECCC WATFLOOD, NOAA-GLERL GLSHyFS, and NOAA NWM are the most skilful input datasets. As noted above, due to its high correlation with NOAA-GLERL GLSHyFS, CCGLHHD is not included in this model run.

Through experimental Run IDs 1 to 42, it is determined that the addition of independent datasets of water balance components decreases model uncertainty. Run ID 44 was developed to determine if this was the result of additional and correlated data (given it is a measure of the same water balance component) or the nature of the Bayesian inference model. Existing datasets were selected at random, permuted and inserted into the model, resulting in numerous additional, feasible, but uncorrelated time series. This was carried out for over-lake precipitation (5 time series were added), over-lake evaporation (5 time series were added), and runoff (4 additional time series). The result was no additional decrease in model output uncertainty, which indicates that as

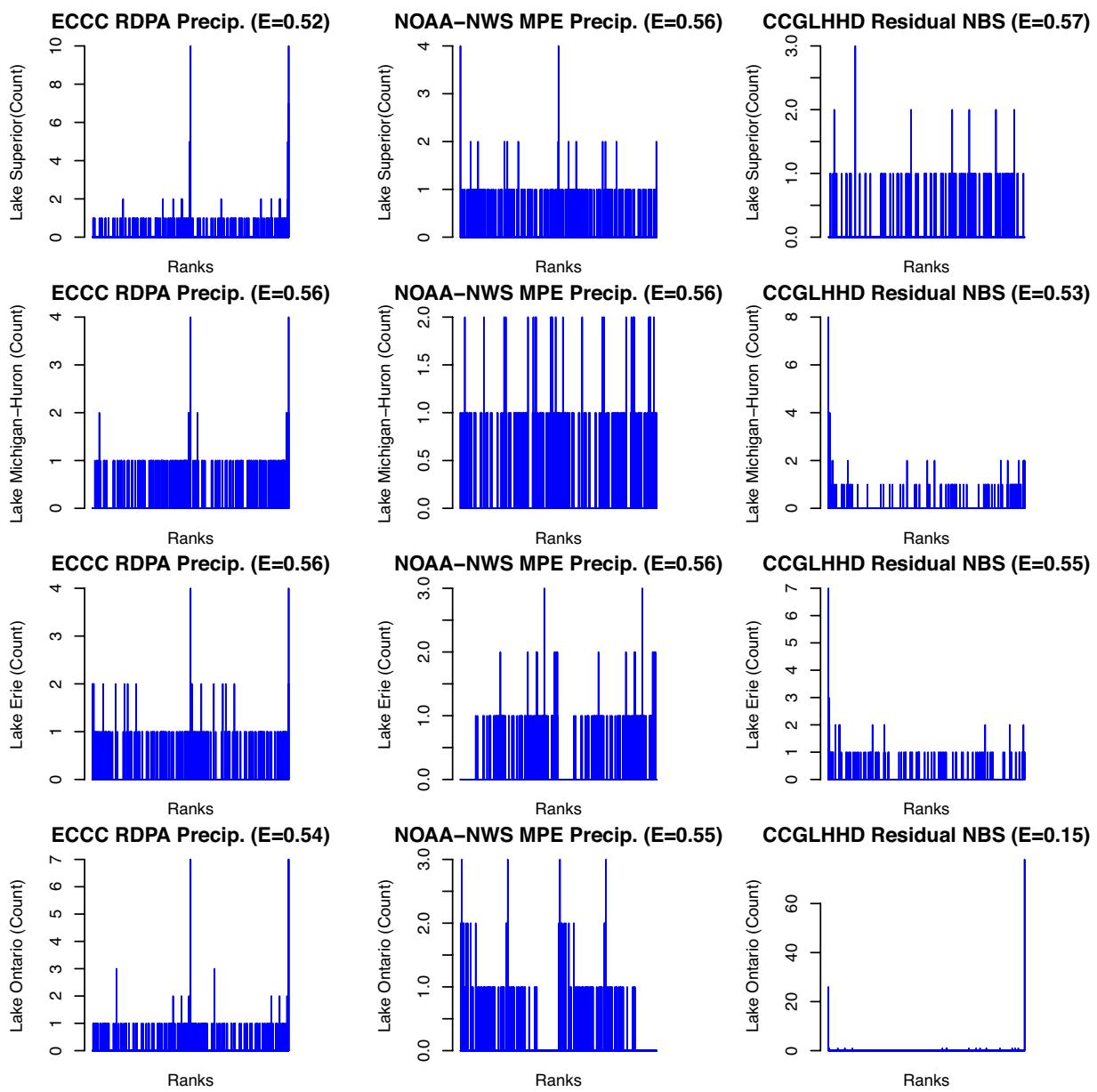


Fig. 7 Rank histograms of L2SWBM over-lake precipitation model output and RDPA, NOAA-NMS MPE, and L2SWBM NBS_c and CCGLHHD NBS_r for Lake Superior, Lake Michigan-Huron, Lake Erie, and Lake Ontario for Run ID 46. Note: E denotes entropy.

additional independent datasets of water balance components are added to the model, there is an associated decrease in model uncertainty.

GLSHyFS has superior model skill in the operational model, which is shown in Figs. 2–4 (and Figs. S1–S9). The intent of Run ID 45 is to determine the model's sensitivity to prior beliefs and to determine if the skill of GLSHyFS is the result of the use of this dataset as priors for the over-lake precipitation, evaporation, and runoff water balance components. Therefore, a repeated operational run was carried out using ECCC RDPA as the over-lake precipitation prior, GLSHyFS for over-lake evaporation, and ECCC WATFLOOD for runoff. Note that no suitable alternative to GLSHyFS is available for over-lake evaporation due to limited periods of record of the alternate datasets. Rank histograms of model output with the updated prior beliefs are provided in Figs. S10–S21, through which it is evident that GLSHyFS continues to have good model skill, and thus confirming that the L2SWBM is not sensitive to the choice of prior belief.

Lastly, the final Run ID 46 is intended to assess the performance of the model with minimal input datasets where two over-lake precipitation, one over-lake evaporation, and one runoff dataset are retained.

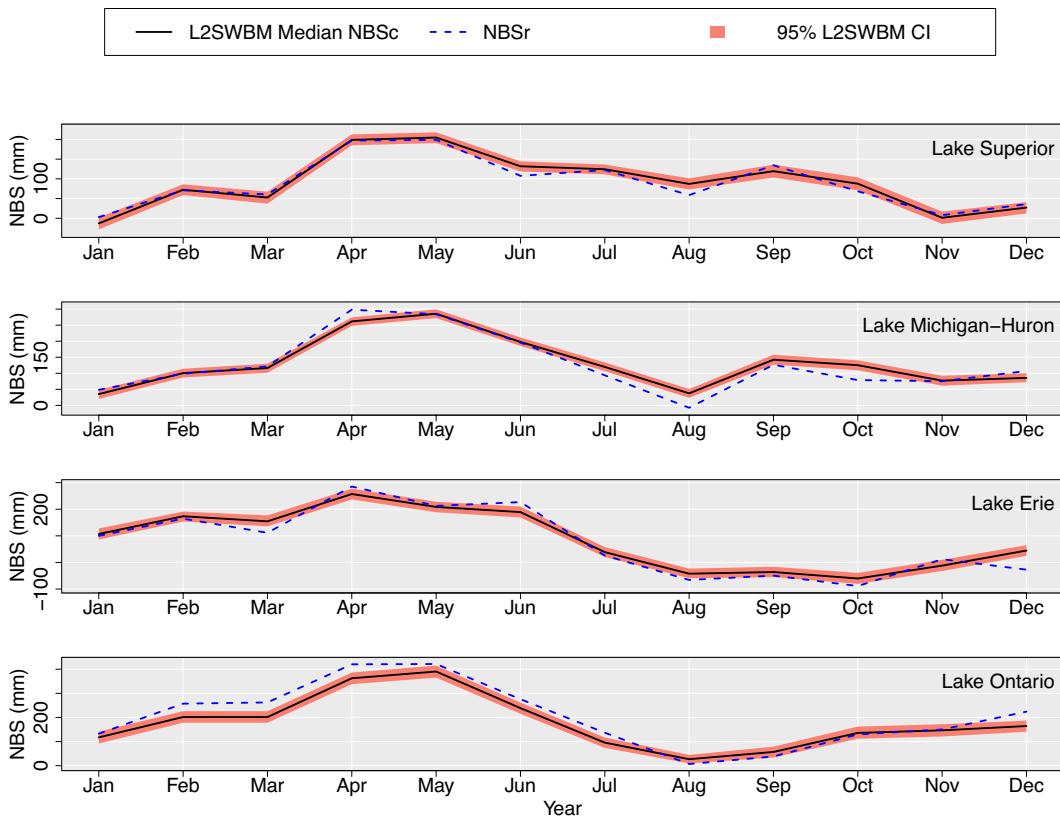


Fig. 8 Comparison of NBS_c from the L2SWBM, NBS_r and the associated 95% credible intervals for 2019.

Data Records

Estimates of water balance components, including over-lake precipitation, over-lake evaporation, and runoff for Lake Superior, Lake Michigan-Huron, Lake Erie, and Lake Ontario are available for download at <https://zenodo.org/records/1388309>⁴⁵. The file size of the data is approximately 350 KB and contains multiple CSV files. Each CSV file contains the 2.5, 50, and 97.5 percentile of the MCMC iterations of the monthly inferences for each lake and water balance component.

Technical Validation

Through the experimental design and associated model runs, the following is observed:

- Consistently high correlations between the CCGLHHD precipitation data and NOAA-GLERL precipitation is the result of the CCGLHHD dataset using GLSHyFS for precipitation input. CCGLHHD precipitation is therefore henceforth removed from the L2SWBM to avoid bias in the output;
- The addition of independent datasets of water balance components into the L2SWBM results in an associated decrease in the uncertainty, as measured by the average size of the credible intervals; and
- The L2SWBM is insensitive to the dataset used to estimate the prior probability distributions.

In consideration of the following results, a final comparison of Run ID 4 (operational model without the CCGLHHD over-lake precipitation) is compared to Run ID 43 (with best model skill) and Run ID 46 (model run with limited datasets). These model runs are assessed for model skill, compared to ECCC RDPA, NOAA-NWS MPE, and NBS_r. Their uncertainty and ability to close the monthly water balance are also assessed. A comparison of model skill for Run ID 4, Run ID 43, and 46 are provided in Figs. 5–7, respectively. Run ID 46 provides slightly higher skill than Run ID 4, however, Run ID 43 provides superior skill to both model runs, most notably for lakes Michigan-Huron and Erie NBS. Model skill is similarly lower for Lake Ontario NBS, owing to the model's low skill in estimating runoff in this basin, which may be the result of error propagation being carried downstream in the model. In light of this, additional research will be carried out to determine the cause of this low model skill, whether it be from the input data or from the L2SWBM.

The difference in output uncertainty between Run IDs 4, 43, and 46 is provided in Table 7. As previously noted, additional datasets of water balance components result in lower model uncertainty. Negative values presented in Table 7 indicate a lower uncertainty in Run ID 4 than in Run IDs 43 and 46, therefore, it is illustrated that there is more uncertainty when the L2SWBM is run with minimal dataset than with additional water balance component estimates for over-lake precipitation, over-lake evaporation, and runoff.

Erie – posterior inferences

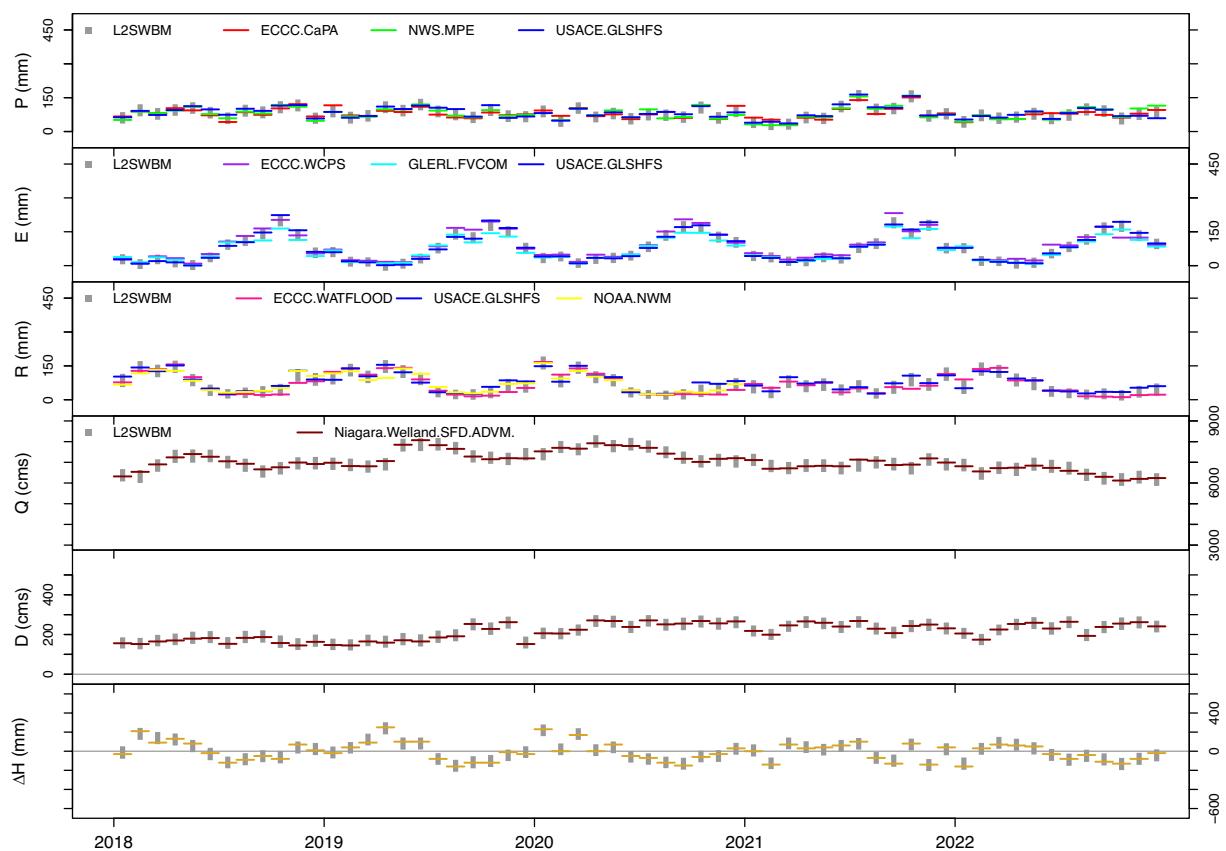


Fig. 9 Overview of L2SWBM credible intervals and input datasets for Lake Erie, which includes results for over-lake precipitation (P), over-lake evaporation (E), lateral tributary inflow (R), connecting channel flow (Q), diversions (D), and the change in lake storage (ΔH).

The final means of comparison between the three model runs is their ability to close the monthly water balance, which is provided in Table 8. Run ID 46, which had limited input data, has an improved capacity for closing the monthly water balance when compared to Run ID 4. There is therefore a trade-off between improved model closure, skill, and increased uncertainty when comparing Run IDs 4 and 46. Run ID 43, which included only models with superior model skill appears to be a good balance between running the L2SWBM with all available datasets (Run ID 4) and with minimal datasets (Run ID 46). There is a slightly decreased capacity of the Run ID 43 to close to the water balance for Lake Michigan-Huron, when compared to Run ID 46, however, this result is small and not statistically significant.

Therefore, Run ID 43 is selected for model configuration and that which is used to develop the final published water balance component datasets. Moving forward, new input datasets to the L2SWBM will be assessed for model skill by the Coordinating Committee before they are added to the model and their impact on model skill, closure, and uncertainty will additionally be evaluated.

Component NBS that closes the water balance is of great benefit to practitioners as it provides reliable forcing data for hydrological modeling. Figure 8 provides a comparison between NBS_c from the L2SWBM for Run ID 43 compared with NBS_r (obtained from CCGLHHD) for 2019, which demonstrates the model's ability to provide water balance components that close the water balance. Although only the median and 95% credible intervals are provided in Fig. 8, it is also important to note that the L2SWBM provides an ensemble of plausible water supply scenarios.

The posterior inferences of the final 1,000,000 iteration model from 2018 to 2022 and their associated 95% credible intervals are provided in Fig. 9 for Lake Erie. Plots of posterior inferences of over-lake precipitation (P), over-lake evaporation (E), lateral tributary inflow (R), connecting channel flow (Q), diversions (D), and change in lake storage (ΔH) for lakes Superior, Michigan-Huron, and Ontario are provided in Figs. S22–S24. In each of the five plots included in Fig. 9, the model's 95% credible intervals are superimposed with the input water balance component datasets. These highlight the differences in input data which are most apparent for over-lake precipitation, over-lake evaporation, and runoff, due to the numerous input datasets for these water balance components. Additionally, the seasonal patterns of the lakes are illustrated in all the presented water balance components in the figure. Of note, the high-water events of 2019 and 2020 are illustrated through peak changes in lake storage in these years.

The L2SWBM will continue to be used operationally by the Great Lakes Coordinating Committee (CCGLHHD), additional datasets of water balance parameters will continue to be added as they become

	Percent Difference (Run ID 4 to 43)	Percent Difference (Run ID 4 to 46)
Lake Superior Diversion (Long Lac/Ogoki)	-0.58%	0.21%
Lake Superior Detention Storage	-3.36%	-17.37%
Lake Superior Over-Lake Evaporation	10.84%	-70.23%
Lake Superior Component NBS	-7.29%	-41.60%
Lake Superior Outflow	-1.72%	0.12%
Lake Superior Over-Lake Precipitation	-36.28%	-39.00%
Lake Superior Lateral Tributary Inflow	-20.72%	-79.09%
Lake Michigan-Huron Diversion (Chicago)	-0.78%	-0.21%
Lake Michigan-Huron Detention Storage	-6.61%	-20.36%
Lake Michigan-Huron Over-Lake Evaporation	8.14%	-75.29%
Lake Michigan-Huron Component NBS	-13.08%	-45.94%
Lake Michigan-Huron Outflow	-0.56%	4.79%
Lake Michigan-Huron Over-Lake Precipitation	-49.57%	-50.53%
Lake Michigan-Huron Later Tributary Runoff	-20.47%	-77.51%
Lake Erie Diversion (Welland Canal and New York State Barge Canal)	0.12%	0.64%
Lake Erie Detention Storage	-4.75%	-16.44%
Lake Erie Over-Lake Evaporation	2.92%	-77.75%
Lake Erie Component NBS	-14.45%	-58.13%
Lake Erie Outflow	-2.03%	-14.70%
Lake Erie Over-Lake Precipitation	-26.86%	-16.22%
Lake Erie Lateral Tributary Runoff	-25.76%	-110.63%
Lake Ontario Detention Storage	-4.18%	-14.25%
Lake Ontario Over-Lake Evaporation	7.40%	-176.51%
Lake Ontario Component NBS	-21.31%	-86.31%
Lake Ontario Outflow	-2.78%	-18.92%
Lake Ontario Over-Lake Precipitation	-28.93%	-16.13%
Lake Ontario Lateral Tributary Runoff	-30.11%	-104.30%

Table 7. Summary of change in uncertainty between experimental Run ID 4 and Run IDs 43 and 46.

	Lake Superior	Lake Michigan-Huron	Lake Erie	Lake Ontario
Monthly Water Balance Closure (Run ID 4)	0.97	0.83	0.94	0.68
Monthly Water Balance Closure (Run ID 43)	0.96	0.88	0.94	0.78
Monthly Water Balance Closure (Run ID 46)	1.00	0.93	0.93	0.78

Table 8. Summary of monthly model closure between experimental Run ID 4 and Run IDs 43 and 46.

available and model improvements will continue. The L2SWBM continues to be valuable tool to provide water balance components and uncertainty in the Great Lakes Basins that reconcile the water balance. Future research will focus on understanding and improving the model skill in Lake Ontario runoff.

Code availability

The code for the L2SWBM model can be accessed on GitHub at the following link: https://github.com/cc-hydrosub/L2SWBM/tree/master/L2SWBM_Nature2023. This provides the current R code used to run the model and a template configuration file used to set model parameters. Also included are the .RData files that include the 2000 plausible water balance scenarios that were established through this study. The L2SWBM uses R programming software and requires 'rjags' package to run the model, as described in the Background and Summary sections.

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Author contributions

N. O'Brien developed and ran the experimental runs, prepared datasets, and led the writing of the manuscript. F. Seglenieks published the datasets. F. Seglenieks, L. Fry, D. Fielder, A.G.T. Temgoua, V. Fortin, and J. Bruxer provided input on experimental run formulation. D. Fielder and A. Temgoua assisted in scripting model improvements. All co-authors provided expert opinion and advice during the preparation on the manuscript.

Competing interests

The authors declare no competing interests.

Additional information

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