Natural Resources Canada | Ressources naturelles Canada

GEOLOGICAL SURVEY OF CANADA
OPEN FILE 8965

A Semiquantitative representation of uncertainty for the 3D Paleozoic bedrock model of southern Ontario

M. Bunn, T.R. Carter, H.A.J. Russell, and C.E. Logan

2023

Canada

GEOLOGICAL SURVEY OF CANADA
OPEN FILE 8965

A Semiquantitative representation of uncertainty for the 3D Paleozoic bedrock model of southern Ontario

M. Bunn[1], T.R. Carter[2], H.A.J. Russell[1], and C.E. Logan[1]

[1]Geological Survey of Canada, 601 Booth Street, Ottawa, Ontario
[2]Geological consultant, 35 Parks Edge Crescent, London, Ontario

2023

Permanent link: https://doi.org/10.4095/331658

This publication is available for free download through GEOSCAN (https://geoscan.nrcan.gc.ca/).

Recommended citation
Bunn, M., Carter, T.R., Russell, H.A.J., and Logan, C.E., 2023. A Semiquantitative representation of uncertainty for the 3D Paleozoic bedrock model of southern Ontario; Geological Survey of Canada, Open File 8965, 1 .zip file. https://doi.org/10.4095/331658

Publications in this series have not been edited; they are released as submitted by the author.

ISSN 2816-7155
ISBN 978-0-660-48079-4
Catalogue No. M183-2/8965E-PDF

ABSTRACT

The Southern Ontario bedrock model is a valuable resource for researchers and practitioners, but its application is subject to uncertainty. To address this issue a semi-quantitative approach to visualize the relative effects of data sparsity for each layer, identify regions where a lack of data support reduces model confidence, and quantify potential errors in data collection and model construction is presented. This analysis summarizes several sources of error, including cartesian position error, error in the vertical position of the formation contact, error between the modelled topographic surface and recorded collar elevations, and error between the modelled formation top surface and formation top picks. Where data is present, these errors are added to provide an approximation of total uncertainty. Where data are not present, uncertainty is approximated as 50% of the range in formation top variation, with an average value of 27.5 m across all layers. The results show that data availability strongly influences the average total error for each layer, with deeper layers exhibiting higher total error due to lower data density. However, this analysis also suggests that the modelled surfaces likely carry errors of less than 5 to 10 m in most regions.

1. Introduction

The southern Ontario lithostratigraphic model (the Model) (Carter et al., 2019, 2021) covers a large area (110,000 km^2) representing the Ontario portion of the Michigan and Appalachian sedimentary basins. The Model was developed to provide a regional 3D perspective of 53 model formations of Phanerozoic sedimentary bedrock with a combined volume of 71,610 km^3 overlying the Precambrian basement. Model layer contact surfaces are primarily controlled by 237,404 contact 'picks' from 21,054 archival borehole records collected for applications other than regional geological modelling (i.e., resource exploration). The majority of this data is from petroleum wells recorded in the Ontario Petroleum Data System (OPDS) relational database which is maintained by the Oil Gas and Salt Resources Library (OGSRL). The petroleum well data is supplemented by 199 stratigraphic tests by the Ontario Geological Survey, 15 measured sections, 3 Michigan petroleum wells, and 30 control points (Carter et al., 2021).

The vast majority of the boreholes (96%) used in model development are clustered within an 80 km buffer of Lake Erie west of the Niagara Escarpment representing roughly 1/3 of the model area. The remaining 4% of boreholes are sparsely distributed across the other 2/3 of the model area. The borehole density drops from 1 borehole in 2 km^2 to 1 borehole in 83 km^2, respectively, for these 2 sub-regions. Borehole coverage also decreases with depth, as fewer boreholes penetrate down to the Precambrian basement. For example, as the majority of boreholes were focused on hydrocarbon exploration in Devonian and Silurian formations, over 90% of boreholes terminate above or within the Upper Ordovician Queenston formation. The 9 older model formation layers below the Queenston are controlled using less than 10% of the boreholes. Data density is illustrated for each geological contact surface in Appendix A.

The sparse borehole coverage in large parts of southern Ontario is mitigated somewhat by the incorporation of bedrock subcrop mapping (incorporated as grided control points at 1 km spacing), measured stratigraphic sections, and control wells (Clark et al., 2020), nevertheless, data support remains highly spatially variable. In addition to the spatial coverage, given the historical nature of the data, standards for spatial location and logging methods (i.e., geophysics) are highly variable. Quality control and quality assurance (QA/QC) on historical data and expert geological guidance can inform model construction in a manner that yields reliable and applicable model results in acknowledgement of these limitations. However, geological modelling, as in all modelling of the natural environment, is an imprecise exercise. Modelling of geological surfaces in the Model is based principally on spatially distributed point data of varying density and accuracy. For the Model, assessment of model confidence is particularly relevant given its regional scale and the use of legacy data in its development. Proper application of such models rely on recognition of the limitations involved in the modelling exercise and their effects on the uncertainty in model results.

2. Sources of Model Uncertainty

Categorization of model uncertainty is foundational to the meaningful application of models. Wellmann et al. (2010) propose a simplified three-category framework well matched to the data available for the Model. In this framework, the Type 1 category represents possible errors in measurement and data collection that result in the data point differing from the true position of the point. For the Model, information of this type is readily available and quantifiable. The Type 2 category represents the ability of a model to represent the geological surface between known data points. Traditionally assessment of this uncertainty has been addressed stochastically by perturbing model inputs following methods developed by Wellmann et al.(2010) and Lindsay et al. (2012). Various methods have been subsequently employed to quantify confidence based on the model realizations generated through perturbation

(Lindsay et al., 2012; Wellmann and Regenauer-Lieb, 2012; Thiele et al., 2016a, 2016b). As will be discussed in further detail in Section 2, the construction methods used for the Model necessitated a different approach, and in this case, Type 2 uncertainty is considered to represent the ability of a single realization of the Model to fit the observed data (i.e., model error). The Type 3 category represents the incomplete knowledge of the geological system, and cognitive bias implicit in geological modelling. This error type can be difficult to quantify (Bárdossy and Fodor, 2001), although is increasingly incorporated for geological models with structural control (Demynov et al., 2019). In sedimentary depositional environments with minor structural control and well documented stratigraphic relationships, such as southern Ontario, implications of this type of uncertainty are expected to be a minor component of overall uncertainty and are not included in this assessment. The sources of uncertainty used in the confidence assessment are summarized in Table 1.

Table 1: Sources Considered in Confidence Assessment

Category and description	**Sources within the Southern Ontario Geological Model**
Type 1:Measurement & Data Error	• Cartesian Position Error • Error in Vertical Position of Geological Contact
Type 2: Limitations in modelling naturally variable surfaces	• Error between Modelled Topographic Surface and Recorded Collar Elevations • Error between Modelled Formation Top Surface and Formation Top Picks

Type 1: Model Uncertainty Based on Measurement and Data Errors

The following sections summarize the various potential sources of error in data measurement or collection. As will be noted for each error, the overall magnitude of error does not necessarily give an indication of overall confidence, as some sources (i.e., horizontal position) have less effect on overall certainty. In each case, an attempt is made to indicate the degree to which the magnitude of error may affect model confidence. Example maps are provided for select surfaces, and maps for the full suite of geological layers are provided in appendices.

Cartesian Position Error

The Cartesian coordinates provided for borehole collars have an associated error that varies with the survey method used to measure the position. In the case of angled boreholes, an additional error on the measurement of borehole inclination and azimuth would affect the location of each individual geological contact. However, in the case of the Model, fewer than 1% of the holes used were found to be inclined, and differences between vertical depth and depth along the hole are small relative to the scale of the model. Given these conditions, a single error estimate is applied to all mapped contacts associated with the hole, representing the horizontal measurement error only. A location accuracy value is recorded in OPDS for each petroleum well location based on the work of Carter and Castillo (2006). This value varies from 1 m to 1000 m, with over 95% of the points being within 200 m of true location (Carter et al., 2019, 2021). Collars with errors greater than 1000 m are excluded from the model. Analysis of the location errors revealed no spatial correlation, and non-Gaussian distributions. To visualize such highly variable and densely spaced data in the absence of spatial correlation, the errors were averaged over 100 km^2 areas for display purposes. As shown on Figure 1, although this error is generally low, it tends to be highest where data is sparse (east of the Niagara Escarpment). In these sparser areas a single collar may be present within the averaging footprint. The model horizontal resolution of 400 m limits the effect of model errors under 200 m on overall confidence; however, the presence of higher errors in low density areas will further enhance uncertainty and contribute to reduced model confidence where there is limited data support. As the location error is generally lower than model resolution (400 m), this error is considered to be negligible, and not carried through the assessment.

Position errors occur with vertical measurement of the borehole collar elevation (the reference point for vertical measurement of formation top depth); however, data to support this type of confidence assessment is unavailable. Select collar elevations have been surveyed using high accuracy GPS. The remainder of the elevations are determined using the provincial DEM and would be subject to higher error. Overall, this error is expected to be on the order of metres. Errors on the order of metres are an order of magnitude less than other vertical position errors discussed below (i.e., *Error in Vertical Position of Geological Contact* and *Error between Modelled Topographic Surface and Recorded Collar Elevations*), as such, collar measurement is not considered a significant component of overall error.

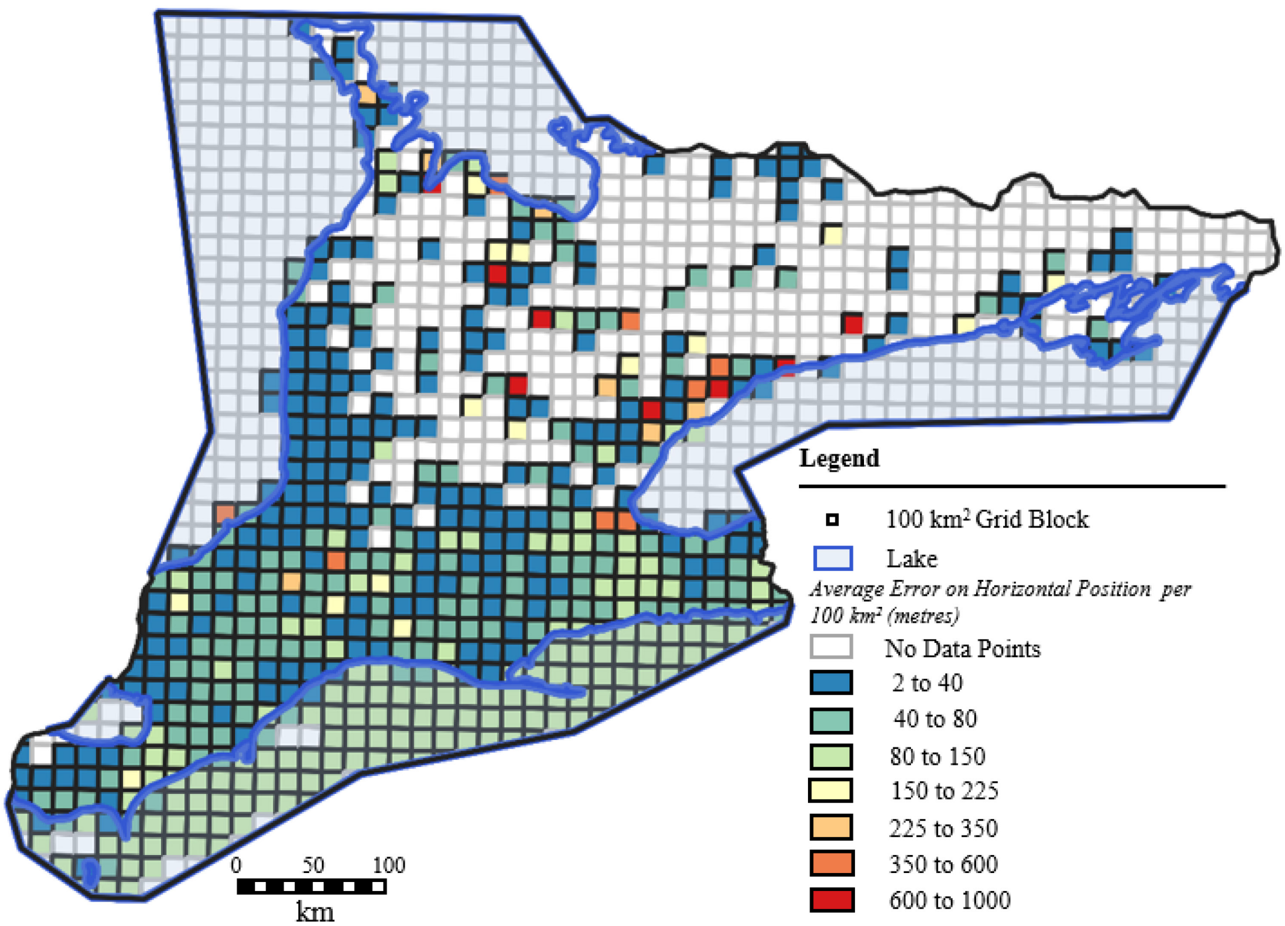

Figure 1: Cartesian Location Error

Error in Vertical Position of Geological Contact

For wells records stored within the OPDS, formation top depths (picks) and calculated elevations are sourced from drilling completion records submitted to the Ministry of Natural Resources and Forests (MNRF) by the well operator. As discussed in Carter et al. (2019) these picks are recorded by both geologists and non-geologists during drilling, and are prone to inconsistency and error, most significantly for formations with gradational contacts or for similar lithological units. To reduce these errors, drill cuttings, samples, geophysical logs, and drill core (if available) are examined by MNRF or OGSRL staff and formation tops are picked based on published standards (i.e, Armstrong and Carter, 2010; Beards, 1967; Carter et al., 2019, 2021). Great efforts have been made to perform this quality assurance and quality control (QA/QC) in support of the Model. At the time of this study (Based on OPDS data dated 12-January-2020), approximately 13% of the OPDS picks used in the model have undergone review by geological staff. This QA/QC is focused on specific regions and formations (see Carter et al., 2019, 2021) and as such the percentage of picks reviewed varies by layer from over 96% complete (D Salt, a unit determined from review only) to only 1% complete (Whirlpool). The following section summarizes the error in both the picks that have undergone QA/QC, and the potential error in picks that have not.

Within the OPDS a QA code is used to indicate the degree of review for each formation top pick. These codes are summarized in Table 3 of Carter et al. (2019), and shown here as Table 2. For picks that have undergone QA/QC the codes range from 1.2 to 2, with higher values indicating both increased skill of the reviewer and increased data confidence. Codes in the range from 1.2 to 1.5 are considered reviewed, meaning that a pick was made, but additional data or review is required. Codes greater than 1.7 are considered confirmed, meaning that the reviewer had sufficient data and there is confidence in the pick. For Codes greater than 1.2 most are confirmed, with only 5% considered reviewed. At this stage in the QA/QC process, the relative reduction in error with increased QA Code is not quantified. Lark et al. (2014) investigated the effect of geological skill in geological contact interpretation for cross-section generation and concluded that skill was a relatively small contributor to overall uncertainty. Bond et al., (2007) conducted a similar analysis of experience in seismic image analysis and found that students were as likely to incorrectly interpret an image as those with more than 15 years of experience. Repeated review by staff of different skill levels would help to quantify this error; however, the magnitude of these errors are expected to be less significant relative to the other components of uncertainty, and are not considered critical to this assessment. For this initial assessment, quantification of picking error has been grouped into those points that have undergone QA/QC (QA Code Greater than 1.1), and those that have not.

Table 2. OPDS quality assurance (QA) codes for formation top picks recorded in the well database (From Carter et al., 2019)

Code	Pick Confidence	Source	Description
2.0 1.9 1.8 1.7	Confirmed	MNRF P. Geo P. Geo OGSRL Geologist in Training or Graduate OGSRL Geology Student	The reviewer had good data—rock cuttings, geophysica logs, or rock cores—and is confident in confirming the pick.
1.5 1.4 1.3 1.2	Reviewed	MNRF P. Geo P. Geo OGSRL Geologist in Training or Graduate OGSRL Geology Student	The reviewer made the best possible pick based on the data available: rock cuttings, geophysical logs, or rock cores; however, more data or review should be considered.
1.0	Not Anomalous	MNRF well records	No geological review but does not cause anomalies in 3 D model
Null	Not Evaluated	MNRF well records	Default value for unedited well records submitted by well operators. No subsequent geological review.
-1.0	Anomaly, requires review	Any	Causing local anomalies when used in 3-D mapping an requires review.
-2.0	Anomaly, unresolvable	Any	Causing local anomalies when used in 3-D mapping bu could not be confirmed or corrected because of an absence of data (rock cuttings, geophysical logs, or roc cores).

For wells that have undergone QA/QC (QA Code greater than 1.1), there is an associated minimum error in the vertical position of the pick based on the transitional nature of formation contacts, the lithology of adjacent units, and the type of data (cuttings, geophysical logs, drill core) available. This information was derived through expert guidance from the OGSRL and is summarized in Table 3. For modelling purposes, several formations have been collapsed into single model layers (e.g. Onondaga- Amherstburg and Decew-Rochester-Lion's Head); for these layers the maximum error from the combined formations was assigned to the model layer picks. To determine the total error on the formation top pick, the the OPDS was referenced to determine the data type used to update the vertical position (i.e., logs or samples), then the error associated the with data type was assigned to the pick. If both data types were available, the data type with the lower error was used.. An additional 1 m of error was added to any hole that was rotary drilled due to the mixing of cuttings and borehole cavings as the sample is brought to surface. The mean error for each model layer ranges from 0.5 m to 10.3 m; with 41 of the 52 layers having errors <2 m, seven layers have mean errors between 2 m and 3 m and 3 have mean errors of >3 m and <10.3 m. There is some correlation between mean error for each layer and the maximum error from Table 3, there is also a dependence on the availability of samples versus logs and the relative utility of each. For example, the Bois Blanc formation can only be reliably picked from samples, with an estimated error of 10 m, whereas Georgian Bay – Blue Mountain has an error of 20 m from samples but only 5 m if logs are available. The mean error for Bois Blanc is 10.3 m, whereas the mean error for Georgian Bay – Blue Mountain is only 6.7 m, as 72% of the boreholes that penetrate the Georgian Bay-Blue Mountain formation are logged. Overall, mean errors in vertical position will be shown to be low relative to other sources of error documented herein.

Table 3: Reliability and Error Estimates for QA/QC Formation Top Picks

Group	Formation(s)	Model Layer	Reliable in Samples	Error from Samples(m)*	Reliable in Logs	Error from Logs (m)
	Overburden	Overburden				
Port Lambton	(unsubdivided)	Port Lambton Group	Y	1	Y	1
	Kettle Point	Kettle Point	Y	0.5	Y	0.3
Hamilton	(unsubdivided)	Hamilton Group	Y	0.5	Y	0.3
	Marcellus	Marcellus	Y	0.5	Y	0.3
	Dundee	Dundee	Y	0.5	Y	0.3
	Columbus	Columbus	Y	1	N	NA
Detroit River	Lucas	Lucas	Y	2	N	NA
	Onondaga	Onondaga-Amherstburg	N	3	N	NA
	Amherstburg	Onondaga-Amherstburg	Y	2	N	NA
	Sylvania	Sylvania	Y	0.5	N	NA
	Bois Blanc	Bois Blanc	N	10	N	NA
	Springvale	Springvale	Y	2	N	NA
	Oriskany	Oriskany	Y	0.5	N	NA
	Bass Islands, Bertie	Bass Islands/Bertie	Y	1	N	NA
	G Unit	G Unit	N	3	Y	0.3
	F Unit	F Unit	Y	1	Y	0.3
		F Salt	Y	1	Y	0.3
	E Unit	E Unit	N	10	Y	0.3
		D Unit	N	5	Y	0.3
	D Unit					
		D Salt	Y	1	Y	0.3
	C Unit	C Unit	Y	1	Y	0.3
	B Unit	B Unit	N	2	Y	0.3
Salina		B Equivalent	N	5	Y	1
		B Salt	Y	1	Y	0.3
		B Anhydrite	Y	1	Y	0.5
	A-2 Unit	A-2 Carbonate	Y	0.5	Y	0.3
		A-2 Salt	Y	0.5	Y	0.3
		A-2 Anhydrite	Y	1	Y	0.5
	A-1 Unit	A-1 Carbonate	Y	0.5	Y	0.3
		A-1 Evaporite	Y	0.5	Y	0.3
Lockport	Guelph	Guelph	Y	1	Y	0.3
	Eramosa	Eramosa	Y	2	N	NA
	Goat Island	Goat Island	N	2	Y	0.3
	Gasport	Gasport	Y	1	Y	0.5
	Decew	Decew-Rochester -Lions Head	N	5	N	1
	Rochester	Decew-Rochester-Lions Head	Y	0.5	Y	0.3
	Lions Head	Decew-Rochester-Lions Head	N	3	N	NA
	Irondequoit	Irondequoit-Rockway-Fossil Hill	Y	1	Y	0.3
	Rockway	Irondequoit-Rockway-Fossil Hill	N	2	N	1
	Merriton	Irondequoit-Rockway-Fossil Hill	N	NA	N	NA
	Reynales/Fossil Hill	Irondequoit-Rockway-Fossil	N	2	Y	0.5
Clinton	St. Edmund	St. Edmund	Y	1	N	0.5
	Wingfield	Wingfield	Y	1	N	0.5
	Dyer Bay	Dyer Bay	Y	1	N	0.5
	Neahga	Neahga	Y	0.5	Y	0.5
	Thorold	Thorold	Y	0.5	Y	0.5
	Grimsby	Grimsby	Y	1	Y	1
Medina	Cabot Head	Cabot Head	Y	0.5	Y	0.3
	Manitoulin	Manitoulin	N	5	Y	1
	Whirlpool	Whirlpool	Y	1	Y	0.5
	Queenston	Queenston	Y	0.5	Y	0.3
	Georgian Bay-Blue Mountain	Georgian Bay-Blue Mountain.	N	20	Y	5
	Collingwood	Collingwood	N	3	Y	1
Trenton	Cobourg	Cobourg	Y	1	Y	0.3
	Sherman Fall	Sherman Fall	N	5	Y	2
	Kirkfield	Kirkfield	N	5	Y	2
	Coboconk	Coboconk	Y	1	Y	0.3
Black River	Gull River	Gull River	Y	1	Y	1
	Shadow Lake	Shadow Lake	Y	0.5	Y	0.3
	Cambrian (unsubdivided)	Cambrian	Y	1	Y	0.5
	Trempealeau	Cambrian	Y	1	Y	0.5
	Eau Claire	Cambrian	Y	1	Y	1
	Mt Simon	Cambrian	N	3	Y	1
	Precambrian	Precambrian	Y	2	Y	2

For formation tops that have not undergone QA/QC, the mean absolute difference between the drilling completion record and the QA/QC pick for each layer can provide an indication of the relative error in the driller picks for each formation. This absolute average difference ranges from 0 m (e.g. Marcellus), meaning that the QA/QC result was consistent with the drilling completion record for all picks, to more than 17 m (Sherman Fall). The magnitude of this error does not appear to be a function of the proportion of picks that have undergone QA/QC. For example, for both Sherman Fall and Marcellus 7% of the picks have undergone QA/QC. More than 22% of the picks for both the B Salt and the Georgian Bay-Blue Mountain have undergone QA/QC, yet B Salt error is 0.3 m while the Georgian Bay-Blue Mountain error is 7 m. These differences may have stronger relation to the overall difficulty in identifying the formation contacts. As summarized in Table 3, Georgian Bay-Blue Mountain can only be identified to within 20 m based on samples, in contrast to within 5 m for Sherman Fall.

To provide an estimate of total potential error for picks that have not undergone QA/QC the mean absolute difference between the drilling completion record and the QA/QC pick was added to the potential error in the QA/QC process based on the availability of samples and logs (From Table 3), and the drilling method. For points not within the OPDS, the mean difference between the geologist and driller picks was applied as an error. This addition is considered conservative as many of the non-OPDS points are picked by geologists and are likely to have a lower overall uncertainty than a driller pick. This error data was combined with the error data for the points having undergone QA/QC to compile the total error in vertical formation position by layer. The average error ranges from 0.6 m (Kettle Point) to 19.0 m (Sherman Fall), with 48 of the layers having less than 5 m in error. Like the XY location error, this error is highly variable between adjacent points and shows limited spatial correlation. To visualize this information, the data points within 100 km^2 cells were averaged and plotted to show relative differences across the model domain. This average error is shown for the top surfaces of Bois Blanc, Springvale, and Gasport formations on Figures 2 through 4 respectively, and for all layers in Appendix B. Also included in Appendix B are histograms for the disaggregated point data used to generate the maps.

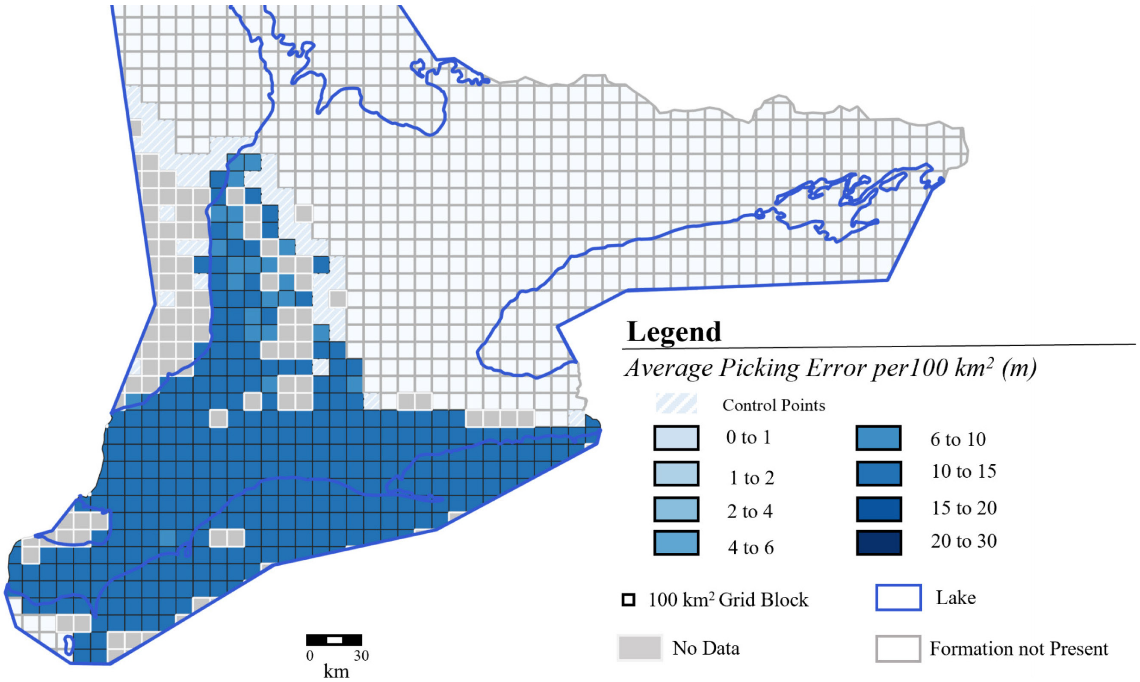

Figure 2 Picking Error on Vertical Position of Top of Bois Blanc Formation (Mean per 100 km²)

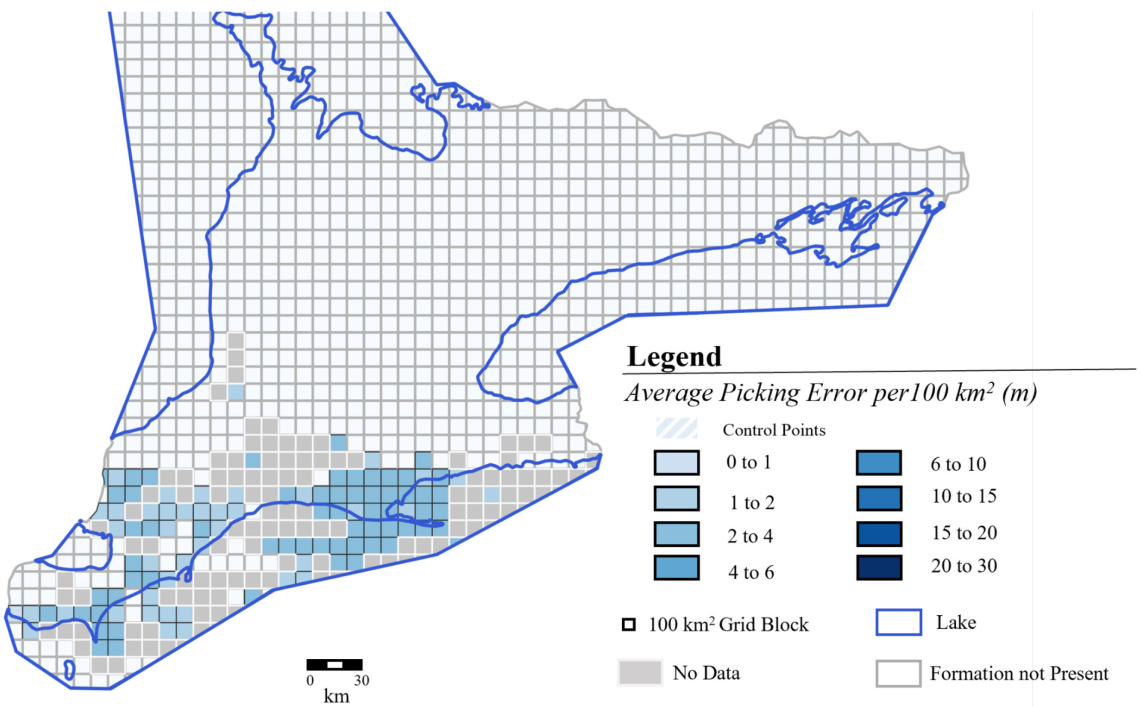

Figure 3 Picking Error on Vertical Position of Top of Springvale Formation (Mean per 100 km²)

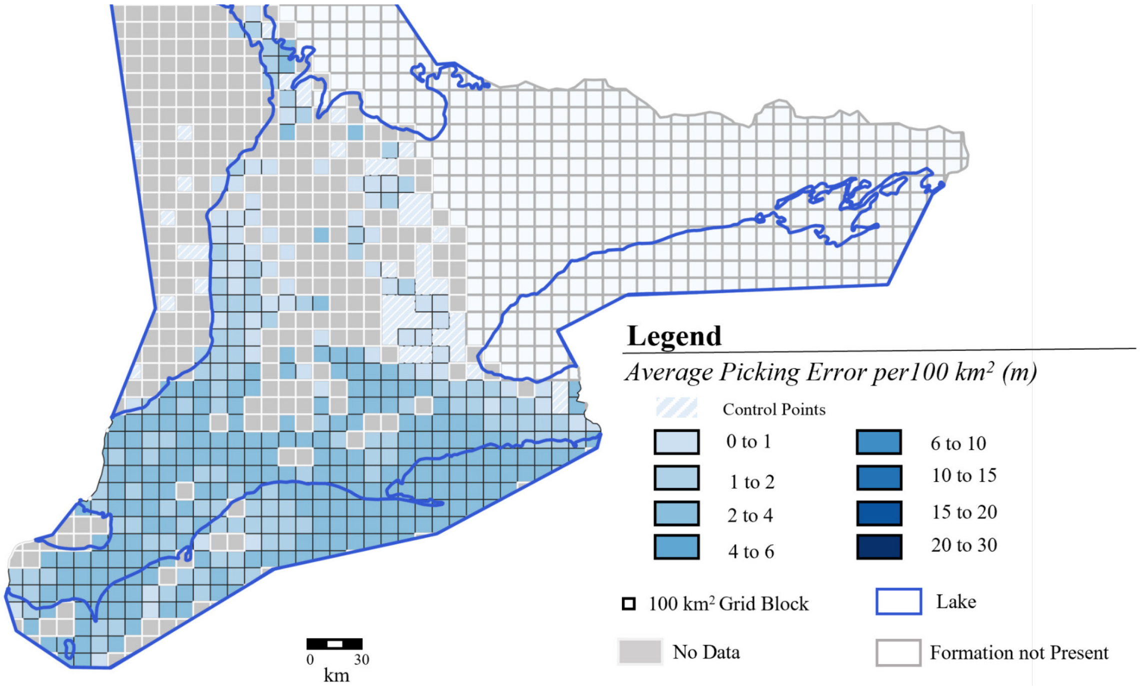

Figure 4 Picking Error on Vertical Position of Top of Gasport Formation (Mean per 100 km^2)

Type 2: Limitations in modelling naturally variable surfaces

Beyond differences between a true formation top and the modelled position resulting from measurement and observational errors, the act of numerically representing surfaces at a plausible resolution results in areas where the model results do not conform exactly to supporting data. This best fit results in a difference between modelled and measured positions. The Model was constructed with a 400 m resolution (Carter et al., 2019, 2021), meaning that modelled surfaces are based on nodes spaced at 400 m. These points are not constrained to available borehole data, and are of lower resolution than available surface topographic information (i.e. the 30 m resolution of the provincial DEM). This resolution effect will result in a discrepancy between both the collar elevation and the modelled topography and a discrepancy between the modelled formation elevation and the data (which is compounded on the topography difference). The following sections quantify the effect of the resolution on model uncertainty, it is noted that increased model resolution was tested for the current model iteration and was not found to be feasible (Carter et al., 2019) given the scope of the model.

Error between Modelled Topographic Surface and Recorded Collar Elevations

Surface topography used in the model is derived from the Ontario Provincial DEM at a 30 m resolution. When imported into Leapfrog the Provincial DEM is mapped to the model grid using an internal averaging process. As a result, smaller scale variability of the topography has been smoothed generating differences between the modelled surface and the input collar elevation.. This difference is used to quantify the effect of horizontal resolution on the vertical position of the surface. Note that boreholes drilled from lake surfaces were removed from this assessment as collar elevations are based on lake level, and the modelled topography incorporates lake bathymetry. For the remaining points, the modelled surface ranges from between 70 m below to 90 m above the recorded collar elevation. The mean difference is -0.7 m indicating that the modelled surface generally falls above the collars. The absolute mean error is 2.54 m. Over 85% of the collar elevations fall within 5 m of the modelled surface, whereas over 95% of the collar elevations fall within 10 m of the modelled surface. This measured difference between model surface and collar was compared to both the surface roughness index and the slope of the topography, with no correlation observed between either of the measures of topographic variability. This result limits the ability to infer potential error between data points, and as such results are presented on Figure 5 as the mean value of the absolute differences for each 100 km^2 cell. Aligned with the general conceptual model of uncertainty, areas with the highest data density tend to have lower mean errors (lower than 3 m). In data sparse areas, the mean error can exceed 20 m due to the increased influence of individual points.

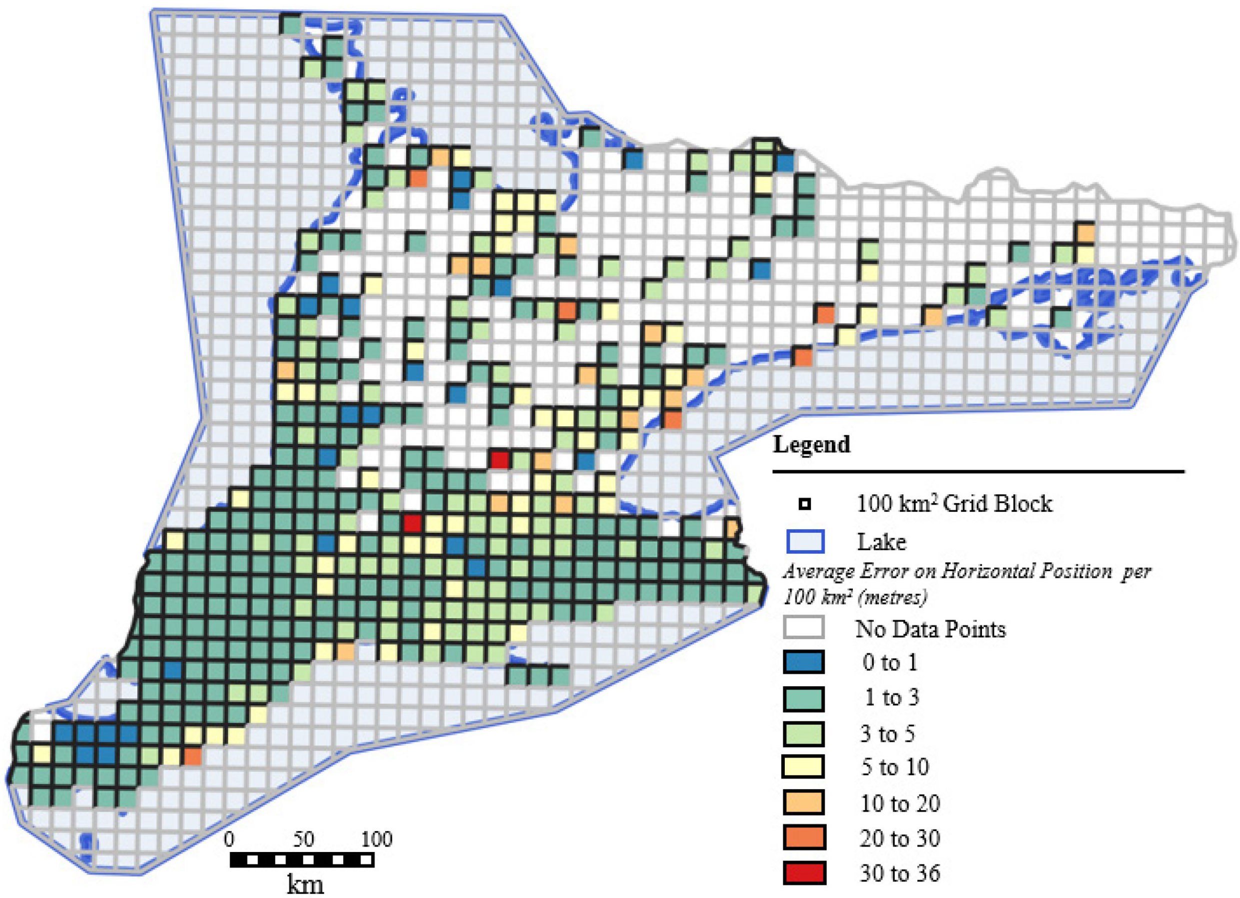

Figure 5: Difference between Collar Elevation and Modelled Topography (Mean per 100 km²)

Error between Modelled Formation Top Surface and Formation Top Picks

As with the topographic surface, the modelled top surface of each geological formation is a best fit surface through available data. Given modelling constraints, parameters, and resolution limitations, the modelled surface is not forced to conform exactly to the data generating small discrepancies termed model error. This model error is compounded by the following factors which contribute to the differential between the data point and the modelled surface:

- The uniformity of the surface: The more smoothly a surface varies, the more likely the model resolution will be sufficient to match the surface variability. Surfaces likely to have stronger variations at scales less than 400 m are likely to show more model error;

- The relative magnitude of the picking error: As a majority of the data points have not undergone the QA/QC process, those formations for which picking error is higher will tend to have larger model errors. Larger picking errors can falsely accentuate differences between adjacent points making it more difficult to fit a modeled surface; and,
- The influence of adjacent surfaces: younging directions and contact types were applied in the modelling process, such that the contact surface avoids all younger borehole lithology intervals (Carter et al., 2019, 2021). This condition can result in automated shifting and manual editing of surfaces to conform to overlying layers, potentially moving surfaces further from data points.

The average error per 100 square kilometer grid cell is shown for the top surfaces of Bois Blanc, Springvale, and Gasport formations on Figures 6 through 8 respectively, and for all formations in Appendix C. Also included in Appendix C are histograms for the disaggregated point data used to generate the maps. Despite the factors listed above, the model error remains moderate with average errors ranging from less than 1 m to 19 m, and 48 layers having an average error of less than 5 m. Errors can exceed 100 m in certain grid cells, such as for the Queenston formation. These larger errors are isolated to single data points within a single layer and do not translate to large errors within adjacent layers, or global discrepancies within the layer. Through the model building process, a Leapfrog process called snapping is used to move the model surface to match the formation data; however, if a point is beyond a certain cut-off distance from the modelled surface, the surface will not be moved, resulting in larger errors such as that for the Queenston formation. This cut-off distance ranges from 4 m to 116 m based on expert guidance (i.e., the snapping distance is higher for Silurian formations with pinnacle reef structures). Formation top picks beyond the set snap range are considered outside the range of natural variability and likely to be spurious data. Additional data would be required to adjust the modeled surface in areas with larger errors to more closely conform to the data. Overall, these larger differences provide more of an indication of the effect of data sparsity, and do not indicate a systematic introduction of uncertainty from the modelling approach. Globally, model results are well matched to the input data.

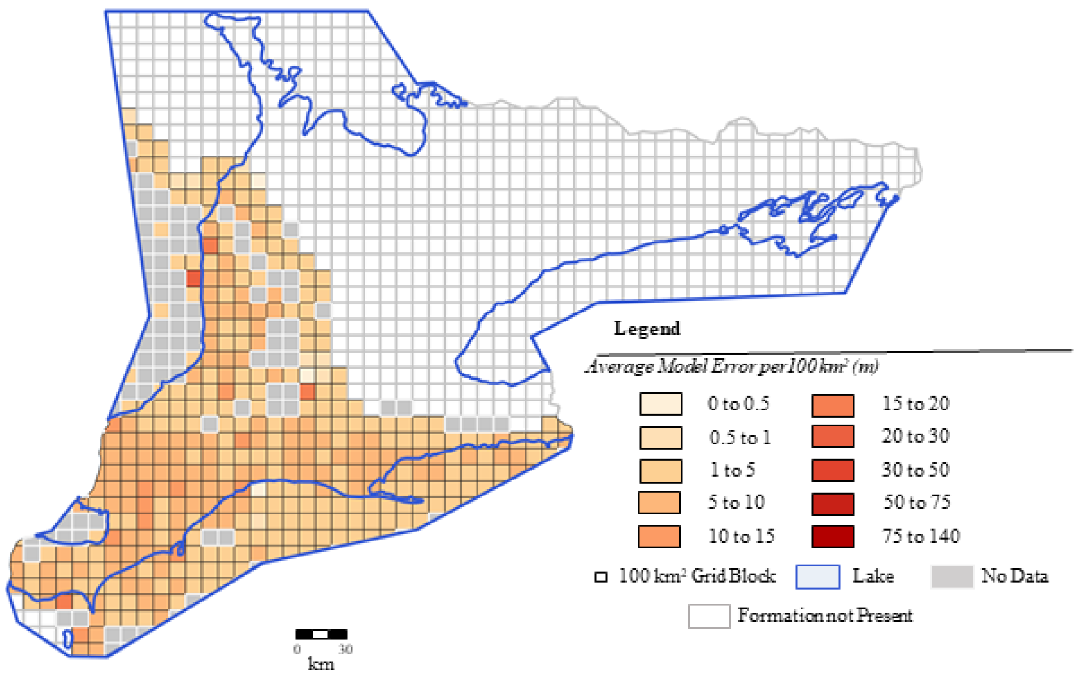

Figure 6 Model Error on Vertical Position of Top of Bois Blanc Formation (Mean per 100 km^2)

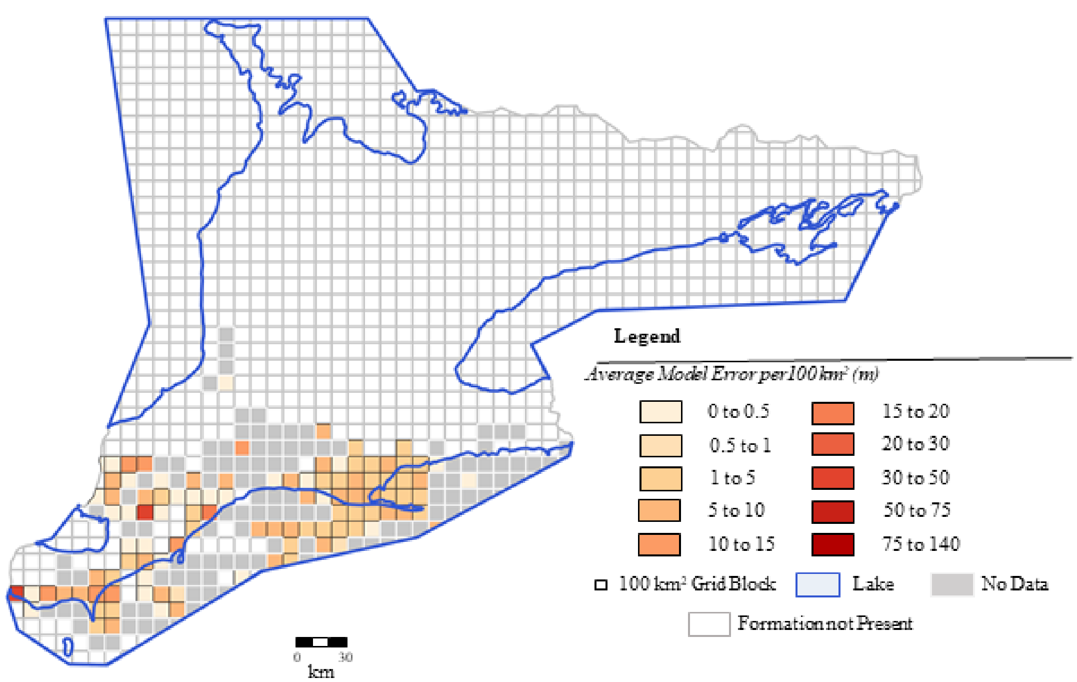

Figure 7 Modelling Error on Vertical Position of Top of Springvale Formation (Mean per 100 km^2)

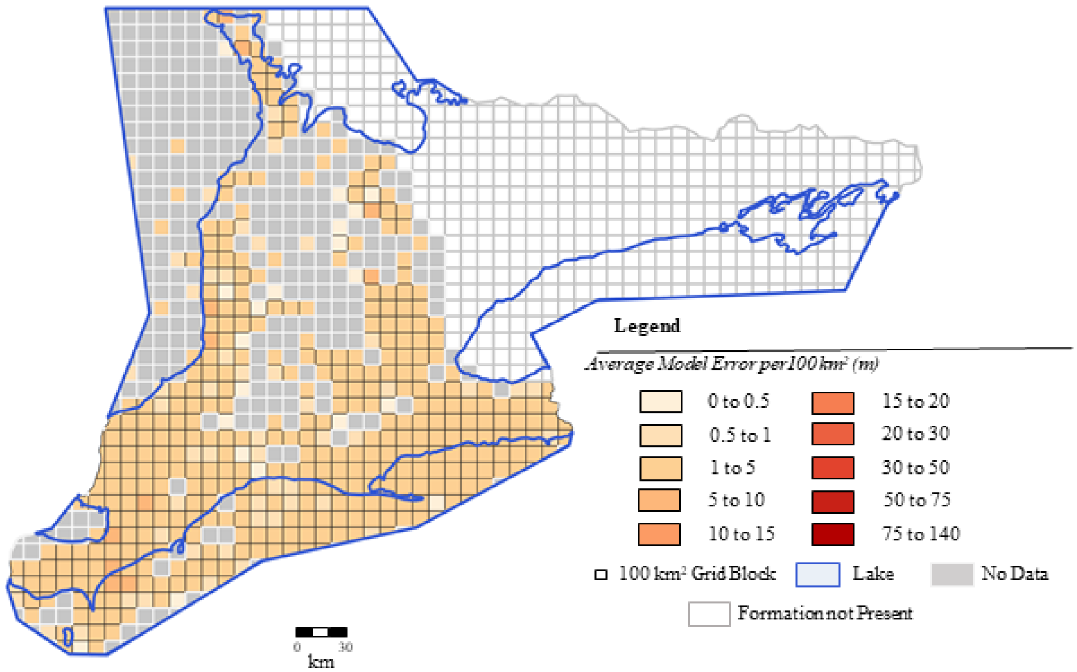

Figure 8 Modelling Error on Vertical Position of Top of Gasport Formation (Mean per 100 km²)

3. Semi-Quantitative Assessment of Total Uncertainty

Due to the nature of the data and the model development process a semi-quantitative approach was taken to quantify error where data was available as detailed above, along with an assessment of potential uncertainty where data support was absent. Combined, these errors represent the total error. Where data is present, the total error was calculated as the sum of each of the average errors per the 100 km^2 grid cells used for data visualization. This addition was completed using the spatial averages rather than the individual points, as not all sources of error are available for each point (i.e., control points do not have an error associated with the vertical position of the formation top), and averages provide a less complex presentation of the totals.

Where the modelled formation top was present within a 100 km^2 grid cell for which there was no supporting point data present, a proxy for total error was calculated based on the range in modelled formation top elevation within that grid cell. The total error assigned to that grid cell was 50% of the range in modelled formation top elevation. This value ranged from 10 m to 40 m with an average of 27.5 m across all layers. Based on the ranges of the model error and picking errors it is unlikely that average errors would exceed this range. As a first approach this assessment of error in the absence of data is considered reasonable, and can be enhanced or validated if additional data becomes available.

The average total error per 100 km^2 grid cell is shown for the top surfaces of Bois Blanc, Springvale, and Gasport formations on Figures 9 to 11, respectively, and for each model layer in Appendix D. Also included in Appendix D are histograms for each surface map. As the Model domain is subdivided into 1191 100 km^2 grid cells for visualization and error calculation, the n value shown on the histograms is representative of the number for grid cells for which the formation is present (out of 1191). This approximation approach highlights the effect of data coverage on model uncertainty, as formation elevation variability generally exceeds any other sources of error. In general, the regions with data display lower potential errors than regions without data, the exception being the isolated areas of certain layers where model error is higher. As data density decreases with formation depth (ranging from more than 60% of the grid cells containing data for the shallowest 20 layers (with the exception of Springvale for which less data is available) to less than 50% for the deepest nine layers (layers below the Queenston formation), there is a related increase in total error with depth. For layers with less than 30% coverage, the mean error is greater than 25 m. For layers with greater than 85% coverage, the mean error is less than 10 m. Some exceptions to this generalized relationship include units such as the Bois Blanc formation, for which the error in the vertical assignment of the formation contact is of similar order to the error assigned in the absence of data, and data coverage does not affect the average layer error.

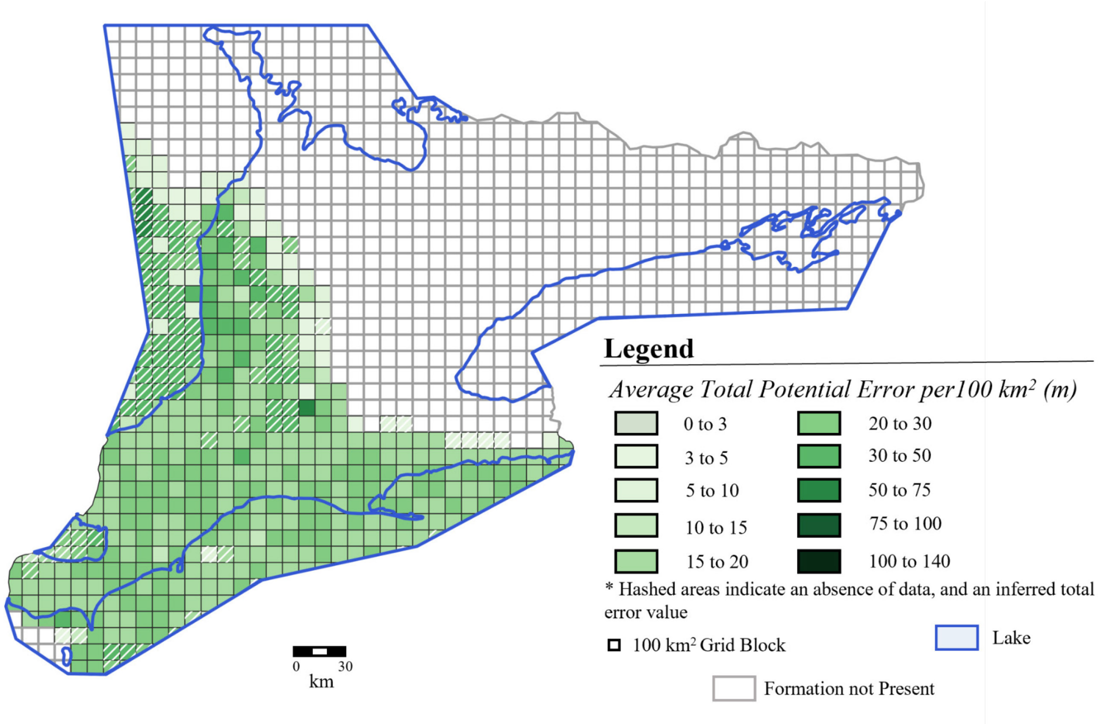

Figure 9 Total Error on Vertical Position of Top of Bois Blanc Formation (Mean per 100 km²)

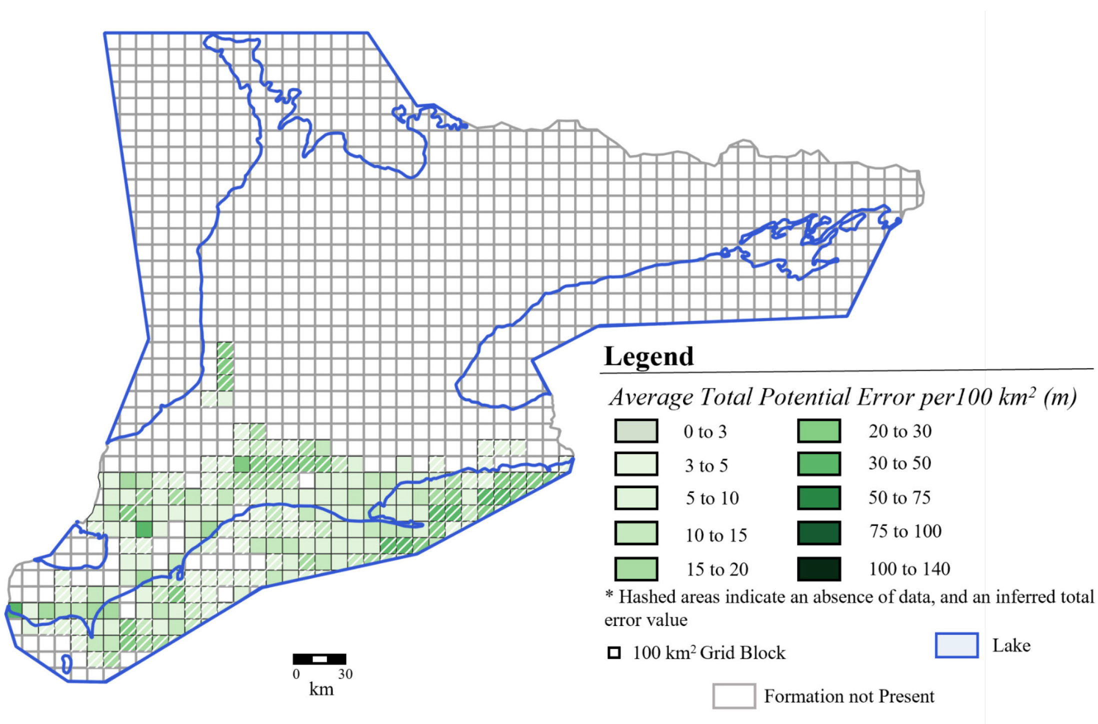

Figure 10 Total Error on Vertical Position of Top of Springvale Formation (Mean per 100 km²)

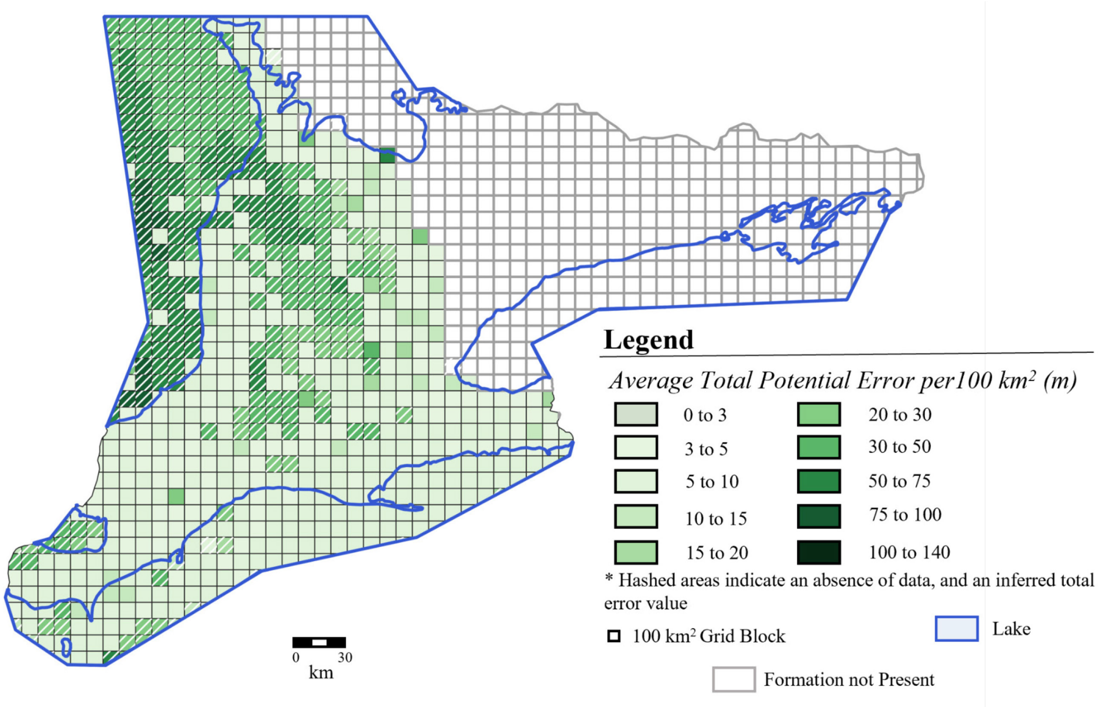

Figure 11 Total Error on Vertical Position of Top of Gasport Formation (Mean per 100 km²)

4. Summary and Future Work

This work is presented as a resource to guide model use and application, and to focus future data validation efforts. This semi-quantitative approach provides a visualization of the relative effect of data sparsity for each layer, and highlights regions for which lack of data support reduces model confidence. In general, errors introduced into the Model related to the assignment of the geological contact are lower than the errors related to the modelling interpolation. When using the Model, the model error layer should also be referenced, as the error can exceed 125 m in isolated regions of certain layers and be quite low otherwise (as related to the cut-off distance discussed above). The total error is more influenced by data sparsity than either of the errors related to the data. Overall, the modelled surfaces likely carry errors of uncertainty of less than 5 to 10 m in most regions. Maps included in the appendices should be used to reference the region and layers from the Model for any practical application of the Model, and uncertainty given greater consideration where errors exceed the required accuracy of the application.

It is anticipated that as the Model is applied for more site specific purposes, local data will vary from the modelled surface. As the scale, scope, and data sparsity of The Model is reduced for regional studies, quantitative methods using cross validation techniques may be used to assess the uncertainty in areas without data support. In addition, as the model is regionalized, kriging or other methods may be used to move away from the 10 km^2 blocks to a more continuous uncertainty visualization. Further, as the Model evolves, there is opportunity for the modelling workflow to be replicated in modelling schemes that support quantitative assessments of uncertainty using Monte Carlo approaches. As new data becomes available, consideration should be given to using this data to assess uncertainty in regions that lacked data in the model build (Carter et al. 2019, 2021). This information would provide a more quantitative assessment of uncertainty for regions without data, and further develop uncertainty estimates in regions with data.

Finally, it is recognized that the impact of uncertainty is a function of the context of the application of the model. As the Model is used in varied contexts from engineering design, exploration, and support of groundwater and integrated groundwater-surface water models the uncertainty in the Model can be carried forward to these applications and should be a foremost consideration for any application of the Model.

Acknowledgements

Internal review by Michael Hillier is much appreciated.

Assistance of Jordan Clark at the Ontario Oil, Gas, Salt and Resources Library was key to the use of the OPDS.

Funding was from the Nuclear Waste Management Organization (NWMO) and the Geological Survey of Canada Groundwater Geoscience Program, Archetypal Aquifer project and Open Geoscience Program Canada 3D project.

APPENDICES

Appendix A - Maps showing data density for each of the 53 model layers

Appendix B - Maps showing error in vertical position of the formation top for each of the 53 model layers
Histograms showing the disaggregated data from the individual data points (n-value represents the number of data points used to generate the model surface)

Appendix C - Maps showing the model error or each of the 53 model layers
Histograms showing the disaggregated data from the individual data points (n-value represents the number of data points used to generate the model surface)

Appendix D - Maps the total error for each of the 53 model layers
Histograms showing the data for the grid cells used to illustrate the data (n-value represents number of cells for which the formation is present out of the 1191 model cells representing the model domain)

REFERENCES

Armstrong, D.K. and Carter, T.R., 2010. The Subsurface Paleozoic Stratigraphy of Southern Ontario, Special volume. Ontario Geological Survey, Mines and Minerals Division.

Bárdossy, G. and Fodor, J., 2001. Traditional and New Ways to Handle Uncertainty in Geology. Natural Resources Research, v. 10, p. 179–187.

Beards, R.J., 1967. Guide to the subsurface Paleozoic stratigraphy of southern Ontario. Ontario Department of Energy Resources Management Paper 67-2, 19.

Bond, C.E., Gibbs, A.D., Shipton, Z.K., Jones, S., 2007. What do you think this is? "Conceptual uncertainty" in geoscience interpretation. Gsa Today 17, 4. https://doi.org/10.1130/GSAT01711A.1

Carter, T.R., Brunton, F.R., Clark, J.K., Fortner, L., Freckelton, C., Logan, C.E., Russell, H.A.J., Somers, M., Sutherland, L., and Yeung, K.H., 2019. A three-dimensional geological model of the Paleozoic bedrock of southern Ontario. Geological Survey of Canada, Open File 8618.

Carter, T.R., Logan, C.E., Clark, J.K., Russell, H.A.J., Brunton, F.R., Cachunjua, A., D'Arienzo, M., Freckelton, C., Rzyszczak, H., Sun, S., and Yeung, K.H., 2021. A three-dimensional geological model of the Paleozoic bedrock of southern Ontario—version 2; Geological Survey of Canada, Open File 8795, 1 .zip file. https://doi.org/10.4095/328297

Clark, J.K., Carter, T.R., Brunton, F.R., Fortner, L., Freckelton, C.N., Logan, C.E., Russell, H.A.J., Somers, M., Sutherland L., and Yeung, K.H. 2020. Improving the 3-D geological data infrastructure of southern Ontario: Data capture, compilation, enhancement and QA/QC; in Russell, H.A.J. and Kjarsgaard, B.A. (eds.), Summary of Southern Ontario Groundwater Project 2014–2019; Geological Survey of Canada, Open File 8536.

Carter, T.R., and Castillo, A.C., 2006. Three-Dimensional Mapping of Paleozoic Bedrock Formations in the Subsurface of Southwestern Ontario: A GIS Application of the Ontario Petroleum Well Database. GIS for the Earth Sciences, Geological Association of Canada.

Demyanov, V., Arnold, D., Rojas, T., and Christie, M., 2019. Uncertainty Quantification in Reservoir Prediction: Part 2—Handling Uncertainty in the Geological Scenario. Mathematical Geosciences, v. 51, p. 241–264.

Lark, R.M., Thorpe, S., Kessler, H., and Mathers, S.J., 2014. Interpretative modelling of a geological cross section from boreholes: sources of uncertainty and their quantification. Solid Earth, v. 5, p. 1189–1203.

Lindsay, M.D., Aillères, L., Jessell, M.W., de Kemp, and E.A., Betts, P.G., 2012. Locating and quantifying geological uncertainty in three-dimensional models: Analysis of the Gippsland Basin, southeastern Australia. Tectonophysics, v. 546–547, p. 10–27.

Thiele, S.T., Jessell, M.W., Lindsay, M., Ogarko, V., Wellmann, J.F., Pakyuz-Charrier, E., 2016a. The topology of geology 1: Topological analysis. Journal of Structural Geology, v. 91, p. 27–38.

Thiele, S.T., Jessell, M.W., Lindsay, M., Wellmann, J.F., and Pakyuz-Charrier, E., 2016b. The topology of geology 2: Topological uncertainty. Journal of Structural Geology, v. 91, p. 74–87.

Wellmann, J.F., Horowitz, F.G., Schill, E., and Regenauer-Lieb, K., 2010. Towards incorporating uncertainty of structural data in 3D geological inversion. Tectonophysics, v. 490, p. 141–151.

Wellmann, J.F. and Regenauer-Lieb, K., 2012. Uncertainties have a meaning: Information entropy as a quality measure for 3-D geological models. Tectonophysics, Modelling in Geosciences, v. 526–529, p. 207–216.