Challenges in hydrologic-land surface modelling of permafrost signatures - Impacts of parameterization on model fidelity under the uncertainty of forcing

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November 21, 2022

Abstract

Permafrost plays an important role in the hydrology of arctic/subarctic regions. However, permafrost thaw/degradation has been observed over recent decades in the Northern Hemisphere and is projected to accelerate. Hence, understanding the evolution of permafrost areas is urgently needed. Land surface models (LSMs) are well-suited for predicting permafrost dynamics due to their physical basis and large-scale applicability. However, LSM application is challenging because of the large number of model parameters and the complex memory of state variables. Significant interactions among the underlying processes and the paucity of observations of thermal/hydraulic regimes add further difficulty. This study addresses the challenges of LSM application by evaluating the uncertainty due to meteorological forcing, assessing the sensitivity of simulated permafrost dynamics to LSM parameters, and highlighting issues of parameter identifiability. Modelling experiments are implemented using the MESH-CLASS framework. The VARS sensitivity analysis and traditional threshold-based identifiability analysis are used to assess various aspects of permafrost dynamics for three regions within the Mackenzie River Basin. The study shows that the modeller may face significant trade-offs when choosing a forcing dataset as some datasets enable the representation of some aspects of permafrost dynamics, while being inadequate for others. The results also emphasize the high sensitivity of various aspects of permafrost simulation to parameters controlling surface insulation and soil texture; a detailed list of influential parameters is presented. Identifiability analysis reveals that many of the most influential parameters for permafrost simulation are unidentifiable. These conclusions will hopefully inform future efforts in data collection and model parametrization.

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- 16 **Corresponding author:** Mohamed Abdelhamed (<u>Mohamed.abdelhamed@usask.ca</u>)
- 17 **Running Title**: Parameterization of LSMs for Permafrost
- 18 Keywords: Permafrost, Land surface models, sensitivity, uncertainty, identifiability, Mackenzie19 River Basin.
- 20 Key Points:
- There are significant uncertainties in climate forcing datasets that affect the fidelity of permafrost simulations using Land Surface Models.
- The quality of simulated permafrost signatures is primarily controlled by heat insulation
 and runoff generation parameters.
- Various highly influential model parameters are non-identifiable, leading to significant
 uncertainty in simulated permafrost characteristics.

28 Abstract

29 Permafrost plays an important role in the hydrology of arctic/subarctic regions. However, permafrost thaw/degradation has been observed over recent decades in the Northern Hemisphere 30 31 and is projected to accelerate. Hence, understanding the evolution of permafrost areas is urgently needed. Land surface models (LSMs) are well-suited for predicting permafrost dynamics due to 32 their physical basis and large-scale applicability. However, LSM application is challenging 33 because of the large number of model parameters and the complex memory of state variables. 34 Significant interactions among the underlying processes and the paucity of observations of 35 thermal/hydraulic regimes add further difficulty. This study addresses the challenges of LSM 36 application by evaluating the uncertainty due to meteorological forcing, assessing the sensitivity 37 of simulated permafrost dynamics to LSM parameters, and highlighting issues of parameter 38 identifiability. Modelling experiments are implemented using the MESH-CLASS framework. 39 The VARS sensitivity analysis and traditional threshold-based identifiability analysis are used to 40 assess various aspects of permafrost dynamics for three regions within the Mackenzie River 41 42 Basin. The study shows that the modeller may face significant trade-offs when choosing a 43 forcing dataset as some datasets enable the representation of some aspects of permafrost dynamics, while being inadequate for others. The results also emphasize the high sensitivity of 44 45 various aspects of permafrost simulation to parameters controlling surface insulation and soil 46 texture; a detailed list of influential parameters is presented. Identifiability analysis reveals that 47 many of the most influential parameters for permafrost simulation are unidentifiable. These conclusions will hopefully inform future efforts in data collection and model parametrization. 48

49 Plain Language Summary

50 Permafrost (frozen ground for at least two years) is one of several elements that control the rate and 51 magnitude of current global warming. Permafrost plays a critical role in the dynamics of water, heat, and 52 carbon over vast areas globally. For more credible climate/hydrology modelling, it is necessary to assess 53 the ability of available models to reliably reproduce observed permafrost characteristics before using 54 them to evaluate future scenarios. Using a land surface model for different permafrost regions in Canada 55 this study examined three challenges: 1) quantifying the impact of uncertainty in climate forcing data on 56 permafrost simulation, 2) identifying the key parameters that control the quality of permafrost simulation, 57 and 3) assessing the appropriateness of current model structures to reproduce observed permafrost characteristics in the context of parameter uncertainty. In selecting a forcing dataset, permafrost 58

59 characteristics exhibited significant trade-offs. The parameters with a large influence on permafrost 60 simulation were identified for the different study areas, but due to model complexity, finding unique 61 values for them was difficult. Several findings were presented to guide further land surface model 62 development, and hence reduce errors in weather/climate modelling.

63 **1 Introduction**

64 Permafrost, defined as ground that stays at or below 0°C for at least two years (Everdingen, 65 1998), plays a central role in the hydrology of arctic and subarctic regions (Dobinski, 2011; Walvoord & Kurylyk, 2016). Permafrost underlies around one-quarter of land in the Northern 66 Hemisphere and one-half of Canada (Obu et al., 2019; Yinsuo Zhang et al., 2008). Several 67 68 studies have reported increased permafrost temperature over recent decades (e.g. Barros et al., 69 2014; Harris et al., 2009; Meredith et al., 2020; Pan et al., 2016) and projected accelerated temperature rises by 2100 (Burke et al., 2020; Lawrence et al., 2012; McGuire et al., 2018). Such 70 71 significant change has major implications for hydrological and biogeochemical cycles (Schuur et 72 al., 2015; Walvoord & Kurylyk, 2016). For instance, permafrost thaw can affect the partitioning 73 of water fluxes and stores, thermokarst formation and land subsidence, wildfire occurrence and 74 other ecosystem changes, and streamflow seasonality (Andresen et al., 2020; Dobinski, 2011; 75 Gibson et al., 2018; Hjort et al., 2018; Kokelj & Jorgenson, 2013; Nelson et al., 2002; Schuur et 76 al., 2015; Walvoord & Kurylyk, 2016). Moreover, permafrost stores twice the amount of carbon in the atmosphere, and its release (in the form of carbon dioxide and methane) is likely to have a 77 78 positive feedback to the global climate and the pace of warming (Burke et al., 2020; McGuire et 79 al., 2018; Schuur et al., 2015).

80 Earth system models (ESMs) are valuable tools for investigating the potential impacts of climate 81 change on hydrologic and atmospheric conditions. They typically represent land surface 82 processes using a land surface model (LSM), which provides lower boundary conditions to the 83 atmospheric processes modelled within an ESM framework. LSMs have advanced significantly 84 over recent decades through extensive improvements in process representation and enhanced resolution (Prentice et al., 2015; Sellers et al., 1997). The coupled simulation of heat and water 85 across the soil-vegetation-atmosphere interface is a critical feature for permafrost as it accounts 86 87 for heat transfer with phase change (Jafarov et al., 2012; Riseborough et al., 2008). Efforts to improve permafrost representation have included (but are not limited to) deeper soil 88 configurations, to eliminate the impact of uncertain lower boundary conditions and provide 89

90 larger thermal memory (Alexeev et al., 2007; Nicolsky et al., 2007), enhanced representation of 91 snow, canopy, and organic soil (including peat and moss) processes that control/regulate thermal 92 insulation of permafrost (Chadburn et al., 2015; Lawrence & Slater, 2008; Wu et al., 2016; Yokohata et al., 2020), and inclusion of vegetation dynamics and carbon-pool processes 93 94 (Chadburn et al., 2015; Melton et al., 2019). These have reduced the biases in climate projections, as shown by Burke et al. (2020). Therefore, LSMs are well-suited for simulating the 95 96 major hydrological processes in permafrost regions, having an appropriate physical basis and being applicable at different assessment scales. 97

98 Despite these advances, building a high-fidelity model is challenging. The paucity of 99 observational data on permafrost hydraulic and thermal regimes limits the representation of 100 permafrost spatial heterogeneity over large domains (Chadburn et al., 2015; Lamontagne-Hallé 101 et al., 2020; Obu et al., 2019). Further, initializing the model prognostic states is problematic. 102 This is commonly achieved by spinning up the models to reach a set of states that are consistent 103 with the 'transient' climate (Abdelhamed et al., 2021; Elshamy et al., 2020; Sapriza-Azuri et al., 104 2018), or based on realistic field observations (e.g. soil moisture and temperature), if available. 105 The spin-up involves forcing the model with a single (actual or synthetic) year or multiple years of meteorological data repeated in a loop many times, or running the model for a long-enough 106 107 transient period. Chen and Dudhia (2001) and Rodell et al. (2005) highlighted the biases in 108 surface energy/water flux partitioning that can be introduced due to the improper initialization of 109 state variables.

110 The structural inadequacy/complexity of LSMs introduces an additional simulation burden. Structural inadequacies of LSMs associated with neglect or oversimplification of permafrost 111 processes (e.g. taliks, thermokarst, and aggradation/degradation) complicates model 112 113 development for permafrost regions, especially those characterized by high heterogeneity (Aas et 114 al., 2019; Devoie et al., 2019; Elshamy et al., 2020). Furthermore, current LSMs have many 115 significant process interactions and contain a large number of free parameters (Prentice et al., 2015). While most of these parameters have a physical meaning, they are usually interpreted and 116 117 measured at point-scale. In the model they serve as "effective parameters" intended to represent 118 the spatial heterogeneity of the system, and therefore, their feasible ranges can be wide and lead to unrealistic model simulations (Haghnegahdar et al., 2017). In conjunction with the improved 119

realism of process representation in LSMs/ESMs, model complexity and dimensionality have increased considerably, making such models more prone to issues of parameter non-uniqueness (Beven, 2006; Guillaume et al., 2019; Prentice et al., 2015). In general, the development and testing of LSMs, including in permafrost regions, have historically focused on streamflows (more frequently), ET and soil moisture (less frequently) (Yassin et al., 2017). The credible representation of the thermal dynamics of the soil column in cold regions has received significantly less attention, while it directly controls those other variables.

127 Complex LSMs require a wider spectrum of meteorological variables at finer spatial/temporal 128 scales than simple hydrologic models, which often require limited forcing variables (e.g. 129 precipitation and temperature/evapotranspiration) at daily and basin-averaged scales. The input forcing (e.g. hydro-meteorological data) uncertainty is typically in the range of 10%-40% 130 (McMillan et al., 2018), and failure to consider such critical uncertainty can lead to 131 unrealistic/biased parameter estimation and misleading water/energy balance calculations. Cold 132 133 regions are characterized by sparse observational networks, especially in higher latitudes and altitudes, and suffer from inaccuracies related to cold-climate processes (Asong et al., 2020; 134 135 Wong et al., 2017), which limits the applicability of ground-based observations. On the other hand, remote sensing and model-based forcing products are prone to different sources of 136 uncertainty triggered by data acquisition, processing, rescaling, and imprecisions. Bias-137 correction (e.g. mean-shifting/scaling or quantile mapping) and the number of considered 138 139 meteorological variables collectively play a pivotal role in the quality (and maintaining crosscorrelation structure) of the candidate grid-based forcing dataset. 140

Here, we examine the capability of different gridded climate datasets to reproduce observed 141 permafrost dynamics under model parameter uncertainty, to aid in selection of the best candidate 142 143 dataset and highlight the uncertainty propagated due to external forcing. We endorse the formal 144 application of Global Sensitivity Analysis (GSA) (Razavi et al., 2021) as a cornerstone tool for model development by presenting its value for understanding model behaviour, identifying 145 important parameters and characterizing parameter uncertainty. Further, we investigate the 146 identifiability of model parameters, emphasizing parameters with high sensitivity, to ensure 147 148 model fidelity and underscore the associated structural issues in such models regarding

149	perma	frost simulations. Fig. 1 provides a graphical presentation of the employed methods and
150	expect	ed outcomes of the current study. Our research addresses three specific objectives:
151	1.	Which forcing datasets enable the model to represent important signatures of permafrost
152		dynamics given the uncertainty in model parameters? And do different signatures impose
153		trade-offs in the choice of forcing datasets?
154	2.	Which model parameters are primarily responsible for uncertainty in predicting different
155		signatures of permafrost dynamics? And to what extent will reducing uncertainty in those
156		parameters lead to a reduction of uncertainty in those predictions?
157	3.	Can existing data reduce the uncertainty in those model parameters of primary
158		importance? And which parameters should be the target of future research to reduce
159		uncertainty in predicting permafrost dynamics?

160 The remainder of the article is organized as follows: **Section 2** presents our methods, case study 161 and model implementation. **Section 3** reports the results of the experiments, and the article ends 162 with a summary and conclusions in **Section 4**.



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Fig. 1. A flowchart of the employed methodology and the expected outcomes.

Models, datasets, and methods

166 2.1 Model description

The Modélisation Environmenntale communautaire – Surface et Hydrology (MESH: Pietroniro 167 168 et al., 2007) is selected for this study because it is physically based, suited for large-scale studies, 169 and includes state-of-the-art representation of the dominant cold regions' processes (Pomeroy et al., 2016). MESH is a semi-distributed, grid-based modelling framework consisting of a land 170 171 surface component that quantifies vertical energy/water fluxes (CLASS: Verseghy, 1991, 2000; 172 SVS: Husain et al., 2016), algorithms for lateral movement of surface/subsurface flow 173 (WATROF: Soulis et al., 2000; PDMROF: Mekonnen et al., 2014) and a grid-to-grid hydrologic 174 river routing module (WATFLOOD: Kouwen et al., 1993b). The spatial heterogeneity within each cell is represented by subdividing it into tiles based on land cover, soil type, or slope and 175 176 aspects. Using the Grouped Response Unit concept (GRU: Kouwen et al., 1993a), tiles with the same characteristics (e.g. needleleaf forest on sandy soil) in different grid cells share the same 177 physiographic attributes, which reduces the parameterization burden and facilitates parameter 178 transferability across space (Pietroniro & Soulis, 2003). Fluxes are typically calculated at a half-179 180 hourly time step at the tile-level and aggregated for each cell based on a weighted average of GRU fractions. MESH is driven by seven meteorological forcing variables: precipitation, air 181 182 temperature, specific humidity, barometric pressure, incoming shortwave radiation, incoming 183 longwave radiation, and wind speed. Interested readers are referred to Wheater et al. (2021) for a 184 recent account on model developments and applications.

185 For the current study, CLASS version 3.6 is used as the LSM and WATROF as the runoff generation algorithm. CLASS solves the coupled water and energy balances for a user-specified 186 187 soil column (the default is a three-layer with thicknesses of 0.1m, 0.25m and 3.75m) generalized across the modelled watershed. We used a deeper soil column with a power-function-based 188 189 discretization of layers (see Section 2.4.1). In CLASS, soil parameters, which determine the 190 thermal and hydraulic regimes, are typically tied to soil texture using pedotransfer functions. 191 Each soil layer's temperature and moisture content evolve at each time step based on the solution 192 of coupled water and energy balance equations. The upper boundary condition of CLASS is 193 determined through solving the surface energy and water balance considering overlaying vegetation and snowcover, and the lower boundary condition as either a zero heat flux or a user-194 195 specified geothermal flux at the bottom of the soil column, with free drainage. No lateral

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196	migration of heat or moisture between adjacent cells is currently implemented except through
197	surface routing. CLASS requires 17 prognostic variables for each tile covering different model
198	initial states above the ground (i.e. snowpack, canopy) and underground (i.e. soil moisture (liquid
199	and frozen) and temperature for each layer). Further details are provided in the CLASS manual
200	(Verseghy, 2012).
201	The following permafrost characteristics were extracted from the continuously simulated soil
202	temperature profiles to describe permafrost dynamics (Fig. 2);
203	1) Temperature envelopes (Tmax and Tmin), calculated as the maximum and minimum soil
204	temperature profiles over the year.
205	2) Active Layer Thickness (ALT), which is the maximum depth of the 0°C isotherm over
206	the year, taken from the Tmax envelope (<i>i.e.</i> thaw only).
207	3) Mean Annual Ground Temperature (MAGTp) at the top of permafrost (permafrost
208	table).
209	4) The D epth of the Z ero Annual Amplitude (DZAA), where the Tmax and Tmin envelopes
210	meet within a tolerance of 0.1°C.
211	5) The depth to Permafrost Base (PB), where the Tmax and Tmin envelopes intersect with
212	the 0° C isotherm, noting that the model does not simulate the freezing point depression.
213	6) Thermal offset, which is the difference between the mean annual temperature at the
214	ground surface and the permafrost table.
215	7) Surface offset, which is the difference between the mean annual temperature at the
216	ground surface and mean annual air temperature (MAAT) - divided into a winter offset
217	(Dec to Feb) and a summer offset (June to August).
218	8) Date of maximum thaw, which is calculated from the evolution of the daily temperature
219	profile of each year and is used to indicate the inter-annual variability of thawing/freezing
220	cycles.



Fig. 2. Schematic of the soil column showing variables used to represent permafrost dynamics, modified
 after Abdelhamed et al. (2021).

224 2.2 Area of study

Three representative permafrost sites with distinctive hydroclimatic conditions in Canada are 225 used in this study (Fig. 3): Jean Marie Creek (JMC) underlain by sporadic permafrost, Bosworth 226 227 Creek (BWC) underlain by discontinuous permafrost, and Havikpak Creek (HPC) underlain by 228 continuous permafrost. The sites are located along the main-stem of the Mackenzie River, 229 Northwest Territories, Canada (Fig. 3). The Mackenzie River Basin (MRB) has a drainage area of 1.78 million km² and partially covers the Yukon, British Columbia, Alberta, Saskatchewan, 230 231 and the Northwest Territories. More than 75% of the basin is underlain by permafrost based on the permafrost Map of Canada (Hegginbottom et al., 1995), with 16% continuous permafrost in 232 the far north and northwest, 27% discontinuous permafrost covering the central east-to-west part 233 of the basin, 26% sporadic permafrost to the south of discontinuous permafrost regions, and 10% 234 isolated patches of alpine permafrost in the southwest of the basin in Alberta and British 235 Columbia. The current climate of the basin is characterized as subarctic (*i.e.* cold, no dry season, 236

cold summer) according to the Köppen-Geiger classification (Peel et al., 2007), with warmer summers projected in the south under the RCP8.5 climate change scenario (2071-2100) (Beck et al., 2018). The discontinuous and sporadic permafrost regions are characterized by warm ground temperatures (-2 to 0 $^{\circ}$ C) and the limit of permafrost is expected to shift northward under climate

- change (DeBeer et al., 2016; Yu Zhang et al., 2008).
- 242 The JMC site is dominated by boreal forest (needleleaf) and scattered shrubs on peat plateaux where the permafrost is relatively warm (MAGTp of -0.1° C) with a limited thickness (~ 4m) and 243 relatively shallow active layer (~ 1.5m thick). The available data from the 85-12B borehole (to 244 9.7m depth) spans the period 1986 to 2000, with no records available in the 21st century. The 245 BWC site is mainly covered by boreal forest (needleleaf and broadleaf) with a thickness of 10-246 50m (MAGTp of -1.5°C) and an active layer thickness of about 2m on average. The available 247 observations (Norman Wells pump station (84-1) to 13.6m depth) cover 1985 to 2001, 2012, and 248 249 2015-2016. The HPC site is covered by taiga forest and shrubs where permafrost is cold 250 (MAGTp of -4° C) with a considerable thickness (> 300m) and an active layer less than 1m thick. Temperatures at Inuvik Airport (site 01TC02) borehole (data to 10m depth) were used for HPC, 251 252 with data available from 2008 to 2016. Fig. 4 shows the temperature profiles used here for model evaluation. The sites have different climate conditions with an average annual daily air 253 254 temperature between $-2^{\circ}C$ and $-9^{\circ}C$ and average annual precipitation between 250 and 400 mm yr⁻¹ among the three sites over the 1979-2016 period (**Table 1**). Thermal and geological data are 255 256 available from various Geological Survey of Canada (GSC) reports (Ednie et al., 2013; Smith et 257 al., 2004, 2009, 2010; Smith, Chartrand, Duchesne, & Ednie, 2016; Smith, Chartrand, Duchesne, 258 Ednie, et al., 2016). Further information on the selected experimental sites is available in 259 Elshamy et al. (2020).







Fig. 3. Location of the study area, temperature boreholes, and permafrost classification.

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Fig. 4. Observed temperature envelopes at A) JMC, B) BWC, and C) HPC sites.

Table 1. Comparison of air temperature and precipitation for the three sites using the available	
meteorological stations for the period (1979-2016) - refer to Table 3 for further information on the	he
utilized meteorological stations.	

Site	Station ID	Mean annual air temperature (°C)		Total annual precipitation (mm)	
Site	Station ID	Mean	Standard deviation	Mean	Standard deviation
JMC	2202570 & 2202578	-2.63	1.03	376.69	88.22
BWC	2202800 & 2202801	-5.04	1.02	295.07	64.73
HPC	2202101 & 2202102	-7.80	1.44	235.68	42.88

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269 2.3 Climate forcing

As mentioned earlier, seven meteorological variables are required at a sub-daily time step to 270 drive MESH. The ground-based stations in the neighbourhood of the study area provide hourly 271 observations for air temperature, relative humidity, wind speed and barometric pressure, while 272 total precipitation is provided daily, and longwave/shortwave radiations are not observed. 273 Therefore, ground-based observations are not fully available and a model-based product is 274 needed for the current study. Forcing dataset selection is constrained by the quality of the 275 meteorological estimates and the overlap with the permafrost experimental datasets. As 276 mentioned earlier, the available records are 1985-2016, 1986-2000, and 2008-2016 for BWC, 277

278 JMC, and HPC, respectively; thus, the selected forcing dataset should begin before 1985 to 279 enable model initialization and performance assessment. A few widely-used forcing datasets start 280 prior to the 1980s, such as WFD (WATer and global CHange (WATCH) Forcing data), available from 1901 (Weedon et al., 2011), the Princeton dataset, available from 1901 (Sheffield et al., 281 282 2006), WFDEI (WFD with the ERA-Interim analysis), available from 1979 (Weedon et al., 2014), WFDEI-GEM-CaPA (WFD with the ERA-Interim analysis bias-corrected by GEM-283 284 CaPA), available from 1979 (Asong et al., 2020), and WFDE5 (bias-corrected WFD with the ERA5 reanalysis), available from 1979 (Cucchi et al., 2020). However, the WFD and Princeton 285 datasets were discontinued in 2001 and 2012, respectively. The combined product of the Global 286 Environmental Model (GEM; Côté et al., 1998), atmospheric forecasts and the Canadian 287 Precipitation Analysis (CaPA; Mahfouf et al., 2007) showed considerable agreement with 288 ground observations for the precipitation (Wong et al., 2017), but GEM-CaPA is not available 289 290 prior to 2002 and the most recent version, the Regional Deterministic Reanalysis System (RDRS v2), is currently only available from 2000 to 2017 (Gasset et al., 2021). 291

292 Three forcing datasets are used in this study: WFDEI, WFDEI-GEM-CaPA (denoted WFDEI-293 GC hereafter), and WFDE5. Given that reasonable estimates of precipitation fields were obtained 294 from WFDEI, as shown by Wong et al. (2017) for Canada, and the fact that it is available from 295 1979 with adequate temporal resolution (3 hours), WFDEI has an advantage. However, it has been found to be slightly biased relative to observation over Northern Canada (above $60^{\circ}N$) 296 297 (Asong et al., 2020; Wong et al., 2017). It was therefore bias-corrected with the relatively short 298 but more accurate GEM-CaPA product. However, the 40m estimates of GEM-CaPA (for 299 temperature, humidity and wind speed) were used to bias-correct the surface-based estimates of WFDEI, yielding the WFDEI-GC dataset at a non-surface reference height (40m) that limits its 300 301 applicability for some hydrologic models (Asong et al., 2020) but not MESH. Additionally, the WATCH Forcing Data methodology was applied to the ERA5 reanalysis data derived using the 302 303 sequential elevation and monthly basis correction method in Weedon et al. (2011) for ERA5 304 reanalysis. WFDE5 was multi-variate bias-corrected for a limited number of meteorological variables (precipitation, temperature, and shortwave radiation) using the simple approach of 305 rescaling the monthly average CRU 'Climate Research Unit' (and/or GPCC 'Global 306 307 Precipitation Climatology Center') estimates (Weedon et al., 2014), unlike Asong et al. (2020) 308 who used multi-variate quantile-mapping to correct the bias for the seven meteorological

variables (conserving cross-correlations amongst them). Monte-Carlo (MC) simulations
incorporating the three forcing datasets (*i.e.* WFDEI, WFDE5, and WFDEI-GC) and under the
full range of parameter uncertainty was used to aid in selecting the best performing
meteorological dataset for MESH/CLASS simulations for the period 1979-2016 (refer to Fig. 1
and Section 2.4.3).

314 2.4 Experimental design and implementation

Experiments were designed to assess input uncertainty, model sensitivity and parameter 315 identifiability of MESH in reproducing the observed permafrost conditions at the three sites with 316 317 distinct climatic and geological conditions (Fig. 1). We conducted these comprehensive analyses 318 using the MESH model (Pietroniro et al., 2007; Wheater et al., 2021) for the full set of LSM (i.e. 319 CLASS) parameters, various model configurations, multiple permafrost variables/performance criteria, for three sites in Canada. We use two lenses for parameter analysis: GSA using the 320 321 variogram Analysis of Response Surfaces (VARS: Razavi and Gupta, 2016a) and traditional 322 threshold-based identifiability analysis. The point-scale experiments are adopted from Elshamy et al. (2020) and Abdelhamed et al. (2021), where MESH was utilized for investigating 323 324 permafrost initialization in LSMs. We employed the soil layering scheme proposed by Elshamy et al. (2020) (Table A1), which extends to a depth of 51.24 m and has a fine discretization for 325 326 the upper 2 meters of the soil (9 layers), in line with the observed ALT for the selected sites (Fig. 327 4). The lower boundary condition of the soil column (*i.e.* Neumann-type flux boundary 328 condition), known as the geothermal flux, was set to zero since several studies underscored its 329 limited/negligible impact on the simulated temperatures on a centennial timescale (Hermoso de 330 Mendoza et al., 2020; Lawrence et al., 2008; Nicolsky et al., 2007; Sapriza-Azuri et al., 2018). Initializing MESH state variables (i.e. soil temperature and liquid/frozen contents) was achieved 331 by spinning the first year of the climate record (*i.e.* Oct 1st, 1979 - Sep 30th, 1980) for 1000 332 cycles for each sampled set of parameters, as recommended by Abdelhamed et al. (2021). 333

334

2.4.1 Selection of parameters, variables, and metrics

Regarding MESH parameters, six groups of parameters representing canopy, soil texture, soil permeable depth, drainage, ponding, and snow cover processes were perturbed within their physical ranges to assess their influence on the permafrost dynamics (**Table 2**). The range of the canopy parameters was based on the lookup tables from the CLASS manual (Verseghy, 2012);

339 note that the three sites were parameterized as needleleaf forest, and hence, their canopy parameters have the same ranges of variation. Ponding, drainage, and snow cover parameters are 340 341 identical across the three setups, with ranges taken from previous studies with the same model (e.g. Davison et al., 2016; Haghnegahdar et al., 2017) and textbook values (Dingman, 2015). 342 Regarding SDEP (depth to the bedrock), we used the gridded bedrock depth dataset by 343 Shangguan et al. (2017) to identify the upper limit, while the maximum root depth is used to 344 define the lower limit. Although runoff generation processes (i.e. interflow, surface runoff and 345 drainage from the soil column) are treated as vertical processes, they allow water to exit the 346 system via the lateral horizons, which influences water stores and hence the hydraulic and 347 thermal regime of the system. The last parameter group defines soil texture as sand, clay, and 348 organic matter percentages. Since each soil layer has three descriptive parameters, and each 349 model configuration has 25 soil layers, we grouped layers as appropriate and assigned the same 350 values to each group's parameters. A new parameter, ODEP defining the depth of organic soil 351 layers is introduced to reduce the number of parameters considered in the analysis, reduce 352 353 computational cost, and facilitate a more straightforward analysis. ODEP is sampled over the 354 given range and nudged to layer boundaries. It is used to divide the soil column into two horizons: horizon *i* with high organic content 'ORGM*i*' for all layers above ODEP, and horizon *j* 355 356 with mineral soil texture and no organic content below it. This also prevents unrealistic combinations that could lead to model crashes and strange behaviour. The range of soil texture 357 358 parameters (Sand % and Clay %) is determined from the Soil Landscapes of Canada (SLC) v2.2 359 (Keshav et al., 2019) after the U.S. Department of Agriculture (U.S. Department of Agriculture, 360 1951), while the range of soil organic content 'ORGMi' is identified from the available 361 geological boreholes at each site.

362	Table 2. Parameters and their corresponding ranges for the model GSA for each site. Id (1:13) refers to
363	canopy parameters, Id (14) refers to permeable soil depth, Id (15:20) refers to drainage/runoff parameters,
364	Id (21:26) refers to soil texture/hydraulic parameters, Id (27) refers to snow-cover parameter, and Id
365	(28:29) refers to ponding parameters.

LI	C	up Parameter Unit Description -	JMC/BWC/HPC			
10	Group		Lower limit	Upper limit		
1		LAMX	-	Annual maximum leaf area index	1.5	2.5
2		LAMN	-	Annual minimum leaf area index	0.5	1.5
3		LNZ0	-	Natural logarithm of the roughness length	2	3
4		ALVC	-	Average visible albedo when fully leafed	0.02	0.04
5		ALIC	-	Average near-infrared albedo when fully leafed	0.15	0.23
6	~	CMAS	kg/m ²	Annual maximum canopy mass	10	30
7	(do	ROOT	m	Annual maximum rooting	0.5	2
8	Can	RSMN	s/m	Minimum stomatal resistance	150	250
9	U	QA50	W/m^2	Reference value of incoming shortwave radiation for stomatal resistance formula	20	40
10		VPDA	-	Vapor pressure deficit coefficient for stomatal resistance formula	0.4	0.9
11		VPDB	-	Vapor pressure deficit coefficient for stomatal resistance formula	0.8	1.3
12		PSGA	-	Soil moisture suction coefficient for stomatal resistance formula	75	125
13		PSGB	-	Soil moisture suction coefficient for stomatal resistance formula	2	8
14	Permeable depth	SDEP	m	Soil permeable depth	2	7.06/15.21/20.24
15	off	GRKF	-	The fraction of (horizontal) saturated soil conductivity moving in the horizontal direction	0.001	1
16	un	KSAT	m/s	(Horizontal) saturated surface soil hydraulic conductivity	0.0001	0.5
17	inage/i	DRN	-	Drainage index controls water seepage from the bottom of the soil column	0	1
18	Drai	DD	km/km ²	Drainage density	2	100
19	П	XSLP	-	Estimated average slope of the tile/GRU	0.0001	0.4
20		MANN	-	Manning's roughness coefficient for overland flow generation "n"	0.01	0.15
21		SANDi	%	Percent sand in the soil of layers i	0/13/0	12/30/32
22	ITe	CLAYi	%	Percent clay in the soil of layers i	8/18/28	12/27/42
23	xtu	ORGMi	%	Percent organic matter in the soil of layers <i>i</i>	0	60/30/15
24	il te	SANDj	%	Percent sand in the soil of layers j	0/13/0	12/30/32
25	So	CLAYj	%	Percent clay in the soil of layers j	8/18/28	12/27/42
26		ODEP	m	Depth of the organic soil	0.1	7/1/1
27	Snow cover	ZSNL	m	Min depth to consider 100% cover of snow on the ground surface	0.05	0.5
28	ding	ZPLS	m	Max depth of water allowed to be stored on ground surface for snow-covered area	0.05	0.5
29	Pon	ZPLG	m	Max depth of water allowed to be stored on ground surface for snow-free area	0.05	0.5

ALT, Tmin and Tmax (refer to **Section 2.1** for definitions) were employed to assess the impact of parameter uncertainty on simulated permafrost dynamics under different forcing datasets, model sensitivities, and parameters identifiability. These three variables shed light upon the overall thermal regime using the annual envelopes (Tmax and Tmin), as well as a specific focus 371 on ALT as the most critical and direct aspect used to describe permafrost dynamics. The BIAS 372 and the Mean Absolute Error (MAE) of Tmin, Tmax and ALT were used to assess the quality of 373 permafrost simulation at the annual time-scale. The error metrics were averaged over time (*i.e.* the record length) and vertical space (i.e. column depth for Tmax and Tmin). Although both 374 375 metrics quantify the direct bias in the model residual, MAE avoids the bias compensation that can happen when one year has a positive bias and another a negative bias. Further, in a detailed 376 377 case study on model performance assessment of behavioural parameter sets (Section 3.5), we considered additional permafrost characteristics (*i.e.* DZAA, PB, thermal offset, surface offset, 378 date of maximum thaw) to ALT, Tmax, Tmin (refer to Section2.1 for definitions). 379

380

2.4.2 Global sensitivity analysis

Sensitivity analysis of model parameters (SA) can be beneficial in identifying the main factors 381 382 (e.g. boundary/initial conditions, driving forcing and model parameters) controlling permafrost dynamics and overall model performance. According to Saltelli and Annoni (2010) and Razavi 383 384 and Gupta (2015), SA traditionally serves three primary purposes: 1) ranking parameters' contribution to output variance, 2) filtering parameters with a negligible influence on output 385 386 variance, and 3) mapping parameters' space to locate the regions with a satisfactory performance - exploring causalities between different processes/hypotheses and supporting decision-making 387 388 are among the other benefits of SA (Razavi et al., 2021). Local sensitivity analysis (LSA) and 389 global sensitivity analysis (GSA) are the main categories of SA. LSA explores output variability 390 around a single reference point, which, regardless of its high simplicity and intuitiveness, is not 391 appropriate for complex environmental models due to their non-linearity and significant 392 parameter interactions (Saltelli & Annoni, 2010). In contrast, GSA evaluates model output variability over the entire feasible factor space, where a large sample of input factors is 393 generated and output variation is analyzed (Saltelli & Annoni, 2010). 394

Controlled model experiments (often LSA with discrete factor space) have been integral for diagnosing model structure and validating potential modifications to enhance permafrost simulation in several LSM studies. For instance, Alexeev et al. (2007), Nicolsky et al. (2007), and Lawrence et al. (2008) improved simulated permafrost dynamics in CLM3 by assessing the sensitivity to soil layer geometries and textures. Sapriza-Azuri et al. (2018) also examined the sensitivity of soil column depth to parameters using CLASS LSM. Chadburn et al. (2015),

401 Paquin and Sushama (2015) and Melton et al. (2019) examined the sensitivity of permafrost to 402 various snow parameterizations, which improved the simulated permafrost extent for JULES and 403 CLASS LSMs. Sapriza-Azuri et al. (2018) and Hermoso de Mendoza et al. (2020) also investigated the sensitivity of the evolution of soil temperatures to the geothermal heat flux. 404 405 Chadburn et al. (2015), Melton et al. (2019) and Elshamy et al. (2020) explored the impact of the depth to bedrock on permafrost thermal/hydraulic regimes. Further, sensitivity to major input 406 407 variables and parameters was necessary for developing and diagnosing the NEST model, which integrates the strength of permafrost models with LSMs (Yu Zhang et al., 2003). Lastly, the 408 analysis of permafrost sensitivity to external forcing was central to quantifying the impact of 409 410 input uncertainty and proposing methodological improvements for LSMs (Burke et al., 2020; McGuire et al., 2018; Paquin & Sushama, 2015; Slater & Lawrence, 2013). It is noteworthy that 411 all the abovementioned studies employed SA informally, which has contributed to a variety of 412 LSM diagnosis/development, but the used 'what-if-scenario-based' LSA has often been 413 criticized for not being thorough enough to yield sound decisions/sensitivities (Saltelli & 414 Annoni, 2010). 415

416 This study utilized the variogram analysis of response surfaces framework (VARS: Razavi and Gupta, 2016a). This provides a comprehensive spectrum of sensitivity information as it bridges 417 418 the variance- and derivative-based approaches. For example, it produces sensitivity indices of the 419 two most common GSA approaches, the derivative-based (Morris, 1991) and the variance-based 420 methods (Sobol, 2001), while being more computationally efficient and statistically robust 421 (Becker, 2020; Puy et al., 2021). To summarize global sensitivities, VARS integrates the 422 directional variograms over a given perturbation scale (e.g. 10 %, 30%, and 50%) and produces a set of sensitivity indices called IVARS (Integrated Variograms Across a Range of Scales) 423 424 (Razavi & Gupta, 2016a).

The STAR-VARS implementation (Razavi & Gupta, 2016b) is used here. This sampling strategy first generates star centers randomly using, *e.g.* Latin hypercube sampling, and then using a structured sampling approach generates the points on the star wings. Sampling is implemented with a resolution of $\Delta h = 0.1$ and with 100 star centers, as recommended by Razavi and Gupta (2016b), where star centers were selected using Progressive Latin Hypercube Sampling (Sheikholeslami and Razavi, 2017). This resulted in a total of 26,200 model evaluations (for 29 parameters) for each permafrost site (see Section 2.4.1). The normalized values of IVARS₅₀ (adds up to 100% to a "Ratio of Sensitivity") are used to outline GSA results. This allows straightforward interpretation of sensitivity indices in terms of parameter importance and facilitates a consistent comparison across different metrics and cases. Model crashes due to infeasible combination of sampled parameters were handled by applying a data-filling strategy for the response surface following Sheikholeslami *et al.* (2019).

437

2.4.3 Uncertainty and identifiability analyses

The study employed the Monte-Carlo (MC) procedure (Fig. 1) to assess the impact of parameter 438 439 uncertainty on simulated permafrost dynamics, represented by ALT, Tmin and Tmax. The MC 440 approach has been integral to various model analysis methodologies, such as the Generalized Likelihood Uncertainty Estimation Framework (GLUE: Beven and Binley, 1992), Regional 441 442 Sensitivity Analysis (RSA: Spear and Hornberger, 1980), and Dynamic identifiability analysis (DYNIA: Wagener et al., 2003). MC analysis was also used for multi-objective calibration of an 443 444 LSM (e.g., (Houser et al., 2001)). Commonly, the MC procedure is based on sampling from uniformly distributed input spaces (*i.e.* model parameters). However, the high dimensionality of 445 446 LSMs and the non-linearity of their response require a large number of samples, with high computational cost, especially as we also explore different meteorological forcing sets. To 447 448 reduce the computational burden, a sampling strategy was used that conveys the maximum information from the model-output space with a minimal sample size (Sheikholeslami et al., 449 450 2021), based on the semi-structured parameter sampling scheme of STAR. Thus the STAR-based samples used for sensitivity analysis are also used to propagate the uncertainty of parameters to 451 452 the simulated permafrost characteristics and to study their identifiability.

Parameter identifiability analysis investigates whether it is theoretically possible to have a unique 453 454 parameter set for a given model structure, forcing data, observations, and response surface 455 (objective function). Such analysis is vital to pinpoint sources of uncertainty and reduce them, leading to more credible model simulations (Guillaume et al., 2019). However, traditional 456 applications of parameter identifiability analysis (via dotty plots or boxplots) involve a degree of 457 subjectivity inherent in defining a behavioural threshold (e.g. acceptable performance accuracy 458 459 as represented by a goodness of fit metric) and commonly do not account for parameter interactions. However, the concurrent application of both sensitivity analysis (forward problem) 460

and identifiability analysis (inverse problem) in this case provides more insights into the
parameter estimation over the whole response surface and at the global optimum (Gupta &
Razavi, 2018). In other words, parameter estimation is examined by two different lenses to
allocate and rule out various sources of uncertainty

The sampled parameter sets for each permafrost site were used for uncertainty and identifiability 465 466 analyses to ensure consistency of explored input/output spaces. The uncertainty analysis was implemented to assess the combined impact of input forcing (*i.e.* meteorological data) and model 467 468 parameters. The primary purpose of such analysis is to select the most appropriate forcing 469 dataset that can encapsulate the observations, which can be achieved by examining the 470 cumulative distribution function of the performance metrics. Parameter identifiability analysis was implemented for parameter sets that collectively fulfilled the three behavioural constraints 471 472 (refer to Section 3.4 and Table 6 for a discussion on the selected behavioural thresholds used for 473 identifiability analysis). In other words, the proposed method aims to assess model simulations 474 that satisfy all criteria (ALT, Tmin and Tmax) at once, *i.e.* using a multi-objective identifiability analysis. 475

476 **3 Results and discussion**

477 3.1 Gridded data sets assessment

A basic comparison of the three forcing data sets versus ground truth observation for the mean 478 annual air temperature and total annual precipitation is provided in Fig. 5. The meteorological 479 480 stations used for the comparison are listed in Table 3. Records at 2 stations at each site had to be merged to obtain a record for the analysis period and the overlap was assessed to ensure 481 482 consistency. To facilitate the comparison of WFDEI-GC to other datasets, including ground observations, we applied an adiabatic lapse rate correction since the air temperature is provided 483 at 40m and the ground observation is measured at ~2m height (the blue shading in Fig. 5). 484 WFDE5 and WFDEI yielded similar mean annual air temperatures at HPC and JMC sites, noting 485 486 that the two data sets outperformed WFDEI-GC at JMC and partially at HPC (1979-2005). The 487 interannual variability was perfectly replicated at the JMC site (with a consistent overestimation 488 of 1.25°C), but not at BWC and HPC, while the HPC site has a significant bias prior to 2004 (between 1-2 °C). Further, WFDEI-GC provides the warmest air temperature with an average 489 490 bias of 2°C, 0.2°C, and 1.25°C for the HPC, BWC, and JMC sites, respectively. However,

WFDE5 and WFDEI-GC deliver better estimates for the air temperature at BWC, while WFDEI persistently underestimates temperature values by 1-2°C. It is noteworthy that no single data product outperforms the others for the three sites collectively for the annual air temperature and similarly for monthly/daily temporal levels (figures not shown).

495 In general, the observed interannual variability for air temperature is better captured than precipitation among the three datasets for the whole period of comparison (1979-2016). The 496 497 comparison of total annual precipitation sheds more light upon the issues/problems associated with these grid-based products. WFDEI-GC systematically overestimates the precipitation at the 498 499 three sites, as does WFDE5 with a lesser magnitude but higher inter-annual variability. On the 500 other hand, WFDEI displays a constant total annual precipitation value at HPC and BWC sites for several consecutive years, between 2008-2015 and 2006-2016, respectively. This could be 501 502 attributed to the fact that CRU (which was used to constrain WFDEI) reverts to the monthly 503 climatology when there is no data (Weedon et al., 2014). Even with the good match between 504 WFDEI and ground observations, on average, the lack of interannual variability (repeated years) 505 is critical in assessing permafrost initialization and dynamics, and thus it might not be advisable 506 to use WFDEI in the current analysis. Lastly, both WFDE5 and WFDEI-GC offer similar results for the precipitation with no clear outperformance at the three sites and throughout the window 507 508 of comparison.

Table 3. List of meteorological stations used for evaluating gridded data sets.

Site	Station ID	Latitude	Longitude	Data Availability
LIDC	2202570	68.30	-133.48	1957-2013
HPC	2202578	68.32	-133.52	2003-2021
DWC	2202800	65.28	-126.80	1953-2012
BWC	2202801	65.28	-126.80	2003-2021
NC	2202101	61.76	-121.24	1963-2014
JMC	2202102	61.76	-121.24	2003-2021



Fig. 5. Comparison of WFDE5, WFDEI, and WFDEI-GC to ground truth observations for mean annual air temperature (left column) and total
 annual precipitation (right panel) at A) HPC site, B) BWC site, and C) JMC site. The range of adiabatic lapse rate correction for WFDEI-GC air
 temperatures is displayed via the light blue shading.

514 3.2 Uncertainty analysis

The overarching goal of this section is to select the dataset that behaves well for most metrics 515 516 and sites, and to investigate the associated uncertainty range. The impact of parameter uncertainty under different external forcing datasets is assessed by aggregating each modelled 517 518 permafrost variable into a single error metric. This provides a general perspective on the effect of 519 using (imperfect) forcing datasets on the quality/accuracy of model predictions. A summary of 520 statistical measures of the cumulative frequency distributions (CDFs) for all experiments across the 26,200 model evaluations (Table 4) shows the best-performing dataset for each site and error-521 criterion in terms of distribution mean and range. The candidate forcing dataset should fulfill 522 minimal mean (CDF at a frequency of 0.5) and minimal envelope (range) of variability, noting 523 524 that having the mean of the CDF around zero is an additional criterion for BIAS-based assessments. Entries in **bold** font in **Table 4** correspond to the best climate datasets to replicate 525 permafrost ground observations. It is clear that WFDEI-GC can reproduce observations using the 526 BIAS and MAE error criterion at the three sites, except for Tmax BIAS at the three sites and 527 ALT at the BWC site. Since the Tmax envelopes similarly encapsulate the observations (among 528 the three datasets), with a slight advantage for WFDEI over WFDEI-GC, and ALT is simply a 529 point on the Tmax envelope, the forcing dataset that has superior estimates for Tmin is selected 530 for the rest of the study. Besides, forcing the three sites with the same climate facilitates a 531 meaningful/comprehensive analysis and interpretation of results; using different input data 532 533 products could yield misleading sensitivity and identifiability results. Thereby, we opted to use WFDEI-GC for the detailed analysis of parameter sensitivity and identification. 534

Site	Criterion	WFD	DE5	WFI	DEI	WFDE	EI-GC
	CITICITOR	BIAS	MAE	BIAS	MAE	BIAS	MAE
	Tmin	-7.2 [-8.8:-1.9]	7.5 [1.5:9.3]	-8.2 [-11:-5]	8.8 [4.5:11]	0.8 [-6:-5.5]	2.2 [1:5.8]
HPC	Tmax	2.6 [0.9 :3.5]	3.9 [1.3:4.5]	1.4 [-4:2.2]	3.6 [1.6:4.4]	1.8 [-2:4]	1.7 [0.8:4.2]
	ALT	-1.2 [-1.6:-0.5]	1.3 [0.5:1.8]	-0.9 [-1.2:-0.2]	0.7 [0.2:1.3]	-0.5 [-3:0.5]	0.5 [0.1:3]
	Tmin	-2.9 [-4.5:0.75]	3.4 [1:5.2]	-4.8 [-6.2:2]	5.5 [2.5:7]	0.8 [-3.5:2.5]	2.3 [0.8:3.6]
BWC	Tmax	1.2 [0:2.25]	1.7 [0.7:2.3]	0 [-1.1:0.9]	1.8 [0.8:3.2]	1.6 [-0.7:3.9]	1.5 [0.3:4]
	ALT	-1.5 [-4.2:-0.5]	1.5 [0.4:4]	-1 [-1.4:-0.3]	0.9 [0.3:1.5]	-1.9 [-13:2]	2.1 [0:11]
JMC	Tmin	-2.3 [-3.5:0]	1.4 [0.8:3.3]	-2.2 [-4.2:1.7]	2.3 [0.8:4.2]	0.1 [-3.2:2.4]	0.9 [0.5:2.7]
	Tmax	2 [0.5:4]	2 [1.2:3.9]	1.4 [0.4:3.7]	1.8 [1:4]	2.6 [-0.5:5.7]	2.7 [0.8:5.2]
	ALT	-1.1 [-8:0]	1 [0.2:8]	-0.9 [-6.1:0.5]	0.8 [0:6]	0.2 [-2:1]	0.2 [0:2.4]

Table 4. Summary of PDFs statistical measures (mean [range]) for two performance metrics, three
 permafrost sites, three permafrost variables, and three climate datasets. Entries in bold indicate datasets
 that yield the best model performance.

To gain insight into the associated uncertainty range under different datasets, the CDFs for the averaged BIAS of Tmin are presented in **Fig. 6**, and the CDFs for the averaged MAE of ALT are shown in **Fig. 7** (refer to **Fig. A1** for the CDFs of the averaged BIAS of Tmax). Several points can be observed:

- WFDEI-GC outperforms the other datasets in simulating Tmin at the three sites. A considerable number of parameter sets can replicate the observed Tmin without any bias. Still, the range of uncertainty is relatively large at the HPC site (range ~ $\pm 5^{\circ}$ C) compared to the other sites (range ~ $\pm 2^{\circ}$ C) forced by the same climate dataset. This can be attributed to an unsuccessful bias removal at HPC site and/or incorporating a wider/unfeasible range for model parameters,
- Both WFDE5 and WFDEI produce cooler Tmin (*i.e.* CDF mean < 0°C) at the three sites,
 noting that the site furthest north (HPC) experiences the coldest bias (~ -7°C on average)
 compared to the -4°C and -2°C biases at the other southern sites,
- WFDE5 provides better estimates of Tmin at the three sites compared to the original
 WFDEI; still, WFDE5 is inferior to WFDEI-GC,
- The range of uncertainty of Tmin for BWC and JMC forced by different climate datasets
 is almost identical, of the order of ~4°C. On the other hand, HPC does not depict the
 same behaviour, as both WFDEI and WFDE5 have a range of uncertainty of ~6°C
 compared to 10°C for WFDEI-GC,

- For ALT, WFDEI-GC offers relatively better estimates (MAE) at the HPC and JMC sites. Yet, WFDEI improves the identification of ALT for BWC site (MAE of 0.9m on average that varies around 0.3m and 1.5m) with respect to WFDEI-GC that does not yield better estimates of ALT (MAE 2.1m on average with a large range of variability between 0 and 11m),
- Unlike Tmin, WFDE5 could not improve the ALT simulation compared to the WFDEI;
 both give a biased estimate with a slight advantage for WFDEI (~ 0.3m improvement in
 the MAE of ALT),
- The distribution shape for ALT is not consistent among the three sites, even under the
 same forcing dataset, highlighting the model's non-linearity. On the other hand, unimodal
 and bimodal normal distribution characterize the Tmin case,
- No single dataset can collectively provide satisfactory model simulations (*i.e.* CDF
 encapsulate the observations with a mean of zero) for ALT and Tmin at the three sites.



Fig. 6. Histograms (red bars) and cumulative frequency distributions (black lines) for the BIAS in
simulated minimum annual temperature envelope (Tmin) at A) HPC site, B) BWC site, and C) JMC site
under WFDE5 (left column), WFDEI (middle column), and WFDEI-GC (right column; the Count (left
axis of each subplot) refers to the number of model evolutions.





Fig. 7. Same as Fig. 6, but showing the MAE in simulated active layer thickness (ALT).

578 3.3 Sensitivity analysis

579 This section discusses GSA results based on the ratio of sensitivity (normalized IVARS₅₀). GSA 580 response surfaces were constructed for both the BIAS and MAE of Tmax, Tmin, and ALT. Unfeasible parameter combinations that violate the numerical stability conditions triggered 581 582 crashes of 6%, 1%, and 10% of the model runs for HPC, BWC and JMC, respectively. As noted 583 above, a model emulation-based substitution technique handled these crashes (Sheikholeslami et al., 2019). Bootstrapping was enabled for all GSA experiments, facilitating the assessment of the 584 585 confidence in GSA results, ensuring the stability of the GSA algorithm, and accounting for randomness in sampling variability (refer to Fig. A2 for the reliability of sensitivity indices). 586

Fig. 8 shows that both the BIAS and MAE experiments yield consistent GSA results. For each 587 permafrost variable, the experiments have similar sets of most sensitive parameters in terms of 588 589 their relative ranking, with a minor impact on each parameter's absolute contribution. JMC is an exception in this regard, as the order of the two most influential parameters to ALT switches; the 590 591 BIAS is dominated by ZSNL (26%) followed by SDEP (16%), while the MAE is controlled by SDEP (24%) and ZSNL (21%). Further, some parameters with moderate influence exhibit 592 593 different behaviour/contribution as per the used metric. For instance, the contributions of XSLP 594 and LAMN to BIAS[ALT] at JMC are 10% and 9%, which become 7% and 8% while 595 considering MAE[ALT]. Such slight variation in parameter sensitivity ratio is amplified when calculating the cumulative influence for each family of parameters (Fig. 9 for BIAS experiments 596 597 and for Fig. A3 MAE experiments). For example, the ponding and snow-cover parameters contribute 57% of the variability of Tmin BIAS for HPC site, altering to 47% for MAE, noting 598 599 that the difference is distributed among the other parameter groups. Besides, the two metrics identify the same insensitive parameters throughout all experiments. Thus, we will focus on 600 601 reporting the detailed sensitivity results for one metric, *i.e.* BIAS.

602 ZSNL has generally the most influence ($\sim 20\%$ -55%) on ALT, Tmin, and Tmax sensitivities at the three sites, except Tmax of HPC site, for which ZSNL becomes the third most important 603 604 parameter ($\sim 12\%$). Evidently, the clear agreement among the three sites stresses the importance of surface insulation (represented by ZSNL) in controlling the thawing and freezing fronts' depth 605 606 and its annual temperature value. However, XSLP is the most influential parameter on Tmax 607 sensitivities at the HPC site, contributing ~20% to BIAS[Tmax] variability. Although XSLP is 608 recognized as a hydraulic parameter with no implicit impact on the thermal system, XSLP is crucial in the current 1-D (vertical) simulation because it determines the amount of water exiting 609 610 the soil column via inter/surface flow mechanisms, which (as noted above) updates water stores 611 and hence the hydraulic and thermal regime of the system.

Overall, Tmin is primarily dominated by three parameters, ZSNL, XSLP, and DD, contributing ~70% of the BIAS. The varying contribution of the three parameters is attributed to the combined impact of external forcing and parameter interactions among the sites. For example, compared to the HPC and JMC sites, the influence of ZSNL reduces (from \geq 40% to 30%) at the cost of increasing the effect of DD and XSLP (~15% collectively) at the BWC site. Besides, the cold and dry conditions at HPC make the aerial snow coverage specification more pivotal to the
insulation against heat loss in winter, which controls around half of the variability in Tmin.
Further, the limited precipitation at HPC (247 mm/year) combined with shallower organic depth
(ODEP<1m), little organic content (<15%), and less porosity (higher sand and clay contents)
resulted in damping the impact of drainage and runoff parameters (XSLP and DD).

622 Tmax is highly affected by the amount and extent of accumulated snow (represented by ZSNL) in the previous winter. The magnitude of influence is similar for BWC and JMC sites (\sim 35%), 623 while the impact decreases at the colder HPC site to $\sim 10\%$. This discrepancy is mainly driven by 624 the external climate variables and the range of soil texture parameters, as highlighted earlier. 625 626 Further, LNZ0 (implicitly the vegetation height) controls the simulation of Tmax, most intensely at HPC (~15%) compared to the other sites (~5% BWC and ~2% JMC), noting that LNZ0 affects 627 628 canopy storage, interception, and latent/sensible heat flux partitioning. On the other hand, ORGMi has the utmost impact on Tmax at the JMC site, with a contribution of ~ 45% of the 629 630 BIAS, noting that the other two sites showed less sensitivity to ORGMi (HPC ~ 1% and BWC ~7%). JMC site has a boarder range of perturbation for ORGMi (0-60%) compared to (0-30%) 631 632 BWC and 0-15% HPC) and for ODEP (0.1-7m) compared to (0.1-1m for both BWC and HPC) that match the site characteristics (Ednie et al., 2013; Smith et al., 2004, 2009, 2010; Smith, 633 634 Chartrand, Duchesne, & Ednie, 2016; Smith, Chartrand, Duchesne, Ednie, et al., 2016). In contrast, the opposite case is associated with SDEP, as the upper limit for the JMC site is ~7m, 635 which is significantly shallower than BWC (15.2m) and HPC (20.2m). The three sites share the 636 same lower perturbation limit for SDEP of 2 m, defined from the maximum possible root depth. 637

Although ALT is extracted from Tmax, it does not depict the same sensitivities for all model 638 639 parameters. For instance, SDEP is surprisingly crucial only for ALT, with a relatively negligible 640 impact on Tmin and Tmax. On average, SDEP contributes ~14% of BIAS[ALT] variability at 641 the three sites. Still, ZSNL exerts the most influence on ALT, with a ratio of sensitivity varying between 20% and 28% at the three sites. The other high-to-moderate parameters among ALT and 642 Tmax experiments are identical in ranking but differ in individual contributions, including DD, 643 XSLP, and ORGMi parameters. Notably, both LAMN and LNZ0 play a moderate role in the 644 645 variability of the ALT, which collectively accounts for 10%-15% at the three sites. These two parameters have an almost similar magnitude of contribution for Tmax, with a slightly lower 646

- 647 effect on Tmin (<9%). In general, the outcome of these comprehensive analyses reinforces the
- 648 importance of surface insulation (LNZ0, LAMN and ZSNL) and subsurface regulation of heat by
- 649 soil texture (ODEP and ORGMi), SDEP, and the drainage efficiency of the system (DD and
- 650 XSLP).



Fig. 8. Ratio of sensitivity of IVARS₅₀ for each parameter in all experiments for A) BIAS[Tmin], B) MAE[Tmin], C) BIAS[Tmax], D)
 MAE[Tmax], E) BIAS[ALT], and F) MAE[ALT]. Ratio of sensitivity of a parameter is calculated as the ratio of its respective sensitivity (IVARS₅₀) to the sum of the sensitivity indices of all model parameters (the ratios of sensitivity for the 29 parameter sum to one).

The study shows that a limited number of model parameters dominates the majority of the response surface variation across the selected error metrics and permafrost variables. Thus, in order to reduce the uncertainty in model predictions, it is crucial to identify/fine-tune these few but highly influential model parameters. Field observations and gridded remotely-sensed products provide a feasible approach in this regard (*e.g.* LAI, ORGM, SDEP), but this is not directly applicable/practical for all model parameters (*e.g.* ZSNL). Inference could be needed to relate some parameters to measured ones.

A substantial reduction in the number of free parameters (for model calibration) is achievable by 662 663 fixing the values of insensitive parameters (e.g. to the median of a priori distribution), which 664 reduces model dimensionality and computational cost of model calibration runs. Accordingly, a list of the most influential parameters for different permafrost aspects in MESH/CLASS is 665 provided in Table 5. We report the 'very' important parameters, which have a ratio of sensitivity 666 larger than 10% (similar to Haghnegahdar et al., 2017). Since there are 18 GSA experiments (i.e. 667 668 three sites x three permafrost variables x two performance metrics), the parameters listed in Table 5 summarize the experiments' union at the HPC, BWC, and JMC sites. There are six 'very 669 670 important' model parameters, namely ZSNL, ORGMi, XSLP, DD, SDEP, and LNZ0. Further, as a secondary goal of the sensitivity analysis, the following model parameters are entirely 671 672 insensitive (<1% contribution): ALVC, ALIC, CMAS, GRKF, MANN, DRN, PSGA and PSGB.

673	Table 5. List of important parameters (ratio of sensitivity $\geq 1\%$) of the MESH model based on the global
674	sensitivity analysis for different variables (and error metrics) and overall (union of all). Very important
675	parameters (ratio of sensitivity $\geq 10\%$) are highlighted in bold.

Rank	Tmin	Tmax	ALT	Overall
1	ZSNL	ORGM <i>i</i>	ZSNL	ZSNL
2	XSLP	ZSNL	XSLP	ORGMi
3	DD	XSLP	SDEP	XSLP
4	LNZ0	LNZ0	ORGM <i>i</i>	DD
5	ORGMi	DD	LAMN	SDEP
6	ROOT	LAMN	DD	LNZ0
7	LAMN	SANDi	SANDi	LAMN
8	VPDA	ODEP	ODEP	SANDi
9	KSAT	SDEP	LNZ0	ODEP
10		ROOT	ROOT	ROOT
11		KSAT	SANDj	SANDj
12		CLAYi	VPDA	VPDA
13		SANDj		KSAT
14				CLAYi

In order to better understand the similarities and differences of GSA results across all BIAS 677 experiments, the cumulative impact of each group/family of parameters (see Table 2 and Section 678 2.4.1) is presented by pie-charts in Fig. 9 (refer to Fig. A3 for MAE results). This reveals that 679 model performance at both JMC and HPC sites is mainly dominated by snow cover and 680 drainage/runoff parameters, which collectively contribute ~72% to the variability in 681 682 BIAS[Tmin], noting that the snow cover group has an absolute higher influence (55% for HPC and 45% for JMC). On the other hand, performance at the BWC site is primarily dominated by 683 the same two parameter groups (75%), with a different proportional impact since the 684 drainage/runoff group has more influence (43%) on the simulation of BIAS[ALT]. The ponding 685 686 and permeable depth groups have minimal impact on Tmin throughout all the experiments, contributing to a maximum of 4% of Tmax variability. Unlike Tmin, the three sites depict a very 687 688 different behaviour for Tmax in terms of the controlling group of parameters. For example, HPC is highly sensitive to drainage/runoff and canopy groups (37%+27%), which is not the case for 689

BWC that is dominated by snow cover and drainage/runoff group (35%+25%), nor for the JMC site that is controlled by soil texture and snow cover (50%+33%). The ponding and permeable depth groups have a minimal impact on Tmax for all experiments, with a maximum contribution of 5%. Lastly, the ALT GSA experiments yield relatively identical partitioning of parameters since no single group dominates more than 30% of the BIAS[ALT] variability. The ponding group of parameters has the most negligible impact on ALT ($\leq 2\%$), while the permeable soil depth becomes more influential to ALT than Tmax and Tmin.



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698 699

Fig. 9. Total ratio of sensitivity (based on IVARS₅₀) for each group of parameters (as indicated in Table 2) for the BIAS across all experiments.

700 3.4 Parameter identifiability

This section explores the degree of identifiability of MESH parameters in simulating ALT, 701 Tmin, and Tmax. Instead of presenting identifiability results for each permafrost variable 702 703 separately, we show parameter sets that simultaneously fulfil the behavioural threshold for the 704 three permafrost variables. This reduces the explored response space and focuses on the global 705 maxima regions. Further, instead of screening/selecting the best model runs based on an arbitrary 706 percentage or number of the total simulations (e.g. 10% as in Wagener et al. (2003) or the best 707 five parameter sets as in Houser et al. (2001)), we opted for the traditional approach in which the 708 screening follows predefined thresholds of performance metrics. Employing this technique is not free of subjectivity in defining these thresholds; but we believe that filtering by a performance metric is relatively less subjective, which was applied for the MAE experiments as follows: $\leq 0.3 \text{ m}$ for MAE[ALT], and $\leq 1^{\circ}$ C for MAE[Tmax/Tmin]. However, the experiments depicted a high discrepancy among sites for the BIAS case, making identifying and unifying these thresholds challenging; having a reasonable number of parameter sets was the other criterion in this assessment. Thereby, each site has a set of distinctive behavioural thresholds used for the identifiability analysis of its model parameters, as summarized in **Table 6**.

716 717

Table 6. Summary of behavioural thresholds per site and performance metric and the total number of parameter sets that fulfill such constraints.

Sito	Critorion	E	SIAS	MAE		
Sile	Cinterion	Range	No. of sets	Range	No. of sets	
LIDC	Tmin & Tmax	$\pm 0.5^{\circ}C$	0	≤1°C	7	
HPC	ALT	±0.25m	9	≤0.3m		
DWC	Tmin & Tmax	±0.15°C	24	≤1°C	89	
БWС	ALT	$\pm 0.05 m$	54	≤0.3m		
MC	Tmin & Tmax	±0.25°C	75	≤1°C	12	
JMC	ALT	±0.1m	73	≤0.3m	13	

718

719 The range of behavioural parameter sets for all sites, scaled between zero and one, is shown in 720 Fig. 10 (BIAS case) and Fig. 11 (MAE case). ZSNL, the most influential parameter in most GSA experiments (see Fig. 9), is broadly identifiable (more constrained) among sites with a slightly 721 722 different setting within its feasible range for each site. For instance, employing the MAE as the 723 performance metric, the HPC model has an identifiable range for ZSNL of 0.6-0.8, while BWC and JMC have identifiable ranges of 0.45-0.7 and 0.55-0.95, respectively (Fig. 11). The three 724 725 sites share the same identified normalized ZSNL value of ~0.7 (i.e. equivalent to ZSNL of 726 0.35m) with a high probability of occurrence (*i.e.* darker dots in Fig. 11). However, the analysis at JMC via the BIAS (Fig. 10) reveals a potential issue as the identifiable normalized value for 727 728 the ZSNL was one (*i.e.* upper end of the range), probably highlighting an inadequately defined 729 parameter range and/or other structural non-identifiability for the JMC model setup. Other 730 experiments show similar behaviour of having an identifiable parameter value at the lower or 731 upper limit of the feasible range (e.g. ORGMi of BWC with MAE); still, the proportion of such problematic parameters is insignificant among all experiments. 732

733 Irrespective of the employed performance metric, highly sensitive parameters (shaded in light red in Fig. 10 and Fig. 11) other than ZSNL do not always depict clear identifiability. For 734 735 example, the range of SDEP for the BWC setup covers almost the whole feasible space; 0.1-0.9 via BIAS and 0.1-0.75 via MAE. The HPC setup sustains the same issue of poorly identified 736 737 SDEP, while it is relatively identifiable for JMC. The inability to determine such a critical parameter affects both the thermal and hydrologic simulation of MESH (Elshamy et al., 2020; 738 739 Haghnegahdar et al., 2017). Further, the highly sensitive hydraulic parameters, XSLP and DD, are not well identified, especially the DD parameter for the BWC setup; XSLP is moderately 740 constrained for HPC and JMC via MAE and BIAS, respectively. Further, the range of LNZ0 741 parameter for HPC differs depending on the utilized performance metric; MAE reduces the 742 743 identifiability range (from 0.2-0.9 to 0.3-0.55). Lastly, a negligible impact of the employed 744 metric on the well-identified ORGMi at the JMC site is observed.

Similarly, moderately influential parameters (shaded in light blue in Fig. 10 and Fig. 11) do not 745 746 depict a consistent response to the employed performance metric. For example, the identifiable range of LNZ0 for BWC is 0.5-1.0 and 0.05-0.35 for MAE and BIAS, respectively, highlighting 747 748 the significant impact of the selected metric on the estimated parameter value. However, the 749 behavioural value for the DD parameter for JMC setup does not change with the selected metric. 750 Noting that a clear improvement on parameter identification for the JMC site is achieved when 751 employing the MAE for the filtering/selecting behavioural solutions, including sensitive and 752 insensitive parameters. This site shares the same behavioural solutions among BIAS and MAE 753 experiments (*i.e.* same darker dots in **Fig. 10** and **Fig. 11**), which is not the case for the other two 754 sites. Besides, the rest of the moderately influential parameters are less identified at HPC and BWC, especially LAMN, VPDB, and KSAT. Therefore, not every highly/moderately influential 755 756 parameter is identifiable for all experiments/sites, underlining the potential parameter interaction 757 and non-uniqueness of fluxes/states partitioning, hence the simulated permafrost.



Fig. 10. Summary of parameter identifiability that simultaneously satisfies the ALT, Tmax, and Tmin
performance criteria at A) HPC, B) BWC, and C) JMC sites. The behavioural parameter sets are filtered
by BIAS performance error, where the number of parameter sets is 9, 34, and 75 for HPC, BWC and JMC
sites, respectively; Light red shade refers to a high influential parameter (ratio of sensitivity ≥10%); Light
blue shade refers to moderate influential parameter (10%> ratio of sensitivity ≥1%); Transparent
markers/points are used that get darker when coinciding or overlapping.







769 3.5 Model performance assessment

This section examines different facets of permafrost dynamics for the selected behavioural
solutions based on the MAE metric at the JMC site (*i.e.* 13 parameter sets shown in Fig. 11C).
This model experiment has long permafrost observations (1985-2000) and reasonably

773 identifiable model parameters. In detail, Fig. 12A-D compare the uncertainty envelopes of ALT, 774 MAGTP, PB and DZAA (refer to Section 2.1 for definitions) with respect to their observed 775 counterparts, extracted mainly from available temperature profiles. Although the maximum allowable average deviation from observed ALT was specified as 0.3m, as highlighted in Table 776 777 6, the envelope of variability corresponding to parameter sets that fulfill such conditions fluctuates between 0.3m-1m, broadly encapsulating the observations. The considerable range of 778 779 variability is attributed to employing an aggregated performance metric (MAE in this case) that 780 compresses the dynamical response of the system in time into a single objective function. One way to address such loss of information is by utilizing non-equal weights (or a form of penalty 781 function) while performing the aggregation to constrain the filtering and ensure a behavioural 782 783 solution replicates the observed behaviour. Another solution can be found in studying the identification of model parameters with finer temporal resolution using, e.g., the DYNamic 784 Identifiability Analysis (DYNIA: (Wagener et al., 2003)). However, even such a thorough 785 approach is challenged by the unique nature of permafrost, as most of its descriptive variables 786 787 are annual-based which limits the number of points used to calculate the metrics and are 788 regulated by complicated interactions between surficial, sub-surficial and meteorological drivers.

789 The selected behavioural solutions produced warmer and thinner permafrost, as depicted in Fig. 790 **12B&C.** The simulated MAGTp is consistently higher than observations by around 1°C 791 (uncertainty range: 0.25°C-1.75°C), except for 1996 and 1997, where few parameter sets could 792 capture observed temperatures, noticing that warmer Tmin and/or Tmax reflect such 793 overestimation in permafrost temperature. Similarly, but to a lesser extent, simulated PB is 794 continually underestimated (e.g. two-folds during the 1990s onset) over the simulation period, with an exception at the beginning (1986-1988) and near the end (1995-2000). The envelope of 795 796 PB depicts high interannual variability that is not shown by observations. Lastly, the DZAA is closely captured with an average variance of 1.5m, as shown in Fig. 12D. Noting that DZAA 797 798 plays a pivotal role in simulating permafrost as it assesses the suitability of the selected soil 799 column depth and identifies the presence of permafrost via calculating its corresponding soil temperature (TZAA) (Burke et al., 2020; Sapriza-Azuri et al., 2018). 800

Fig. 12E&F provide the temporal evolution of the BIAS and MAE of Tmax and Tmin, which were aggregated above to assess model uncertainty, sensitivity, and identifiability. Three

distinctive remarks could be drawn for these figures. First, Tmin tends to be mostly colder than observed as indicated by the BIAS sign, while Tmax envelope is generally warmer. Secondly, Tmin depicts a higher uncertainty range and interannual variability compared to Tmax. Lastly, no clear trade-off between Tmax and Tmin was observed while using MAE or BIAS performance criteria due to error compensation. Although ALT is extracted from Tmax, it does not depict identical variance for behavioural model parameters compared to Tmax, which is compatible with sensitivity analysis results in this regard (**Section 3.3**).

810 Fig. 12G presents the temporal evolution of the date of maximum thaw. Remarkably, there is a 811 wide range of uncertainty (100-150 days) for the date, driven by two distinctive clusters of 812 simulations as shown by the solid lines (each one corresponds to a single parameter set) in **Fig.** 12G. Noting that four parameter sets yielded an earlier (questionable to happen) date between 813 814 May (DOY-130) and June (DOY-180) throughout the simulation period, which cannot be verified or falsified due to the unavailability of thaw timing data. In contrast, the other cluster 815 816 simulated the date of maximum thaw more reasonably, with values varying between DOY-250 and DOY-300; the years 1992 and 1993 were an exception as most of the cluster's members had 817 818 earlier max thawing date (~DOY-200). Such a major discrepancy in maximum thaw timing 819 highlights a potential challenge in LSM applications, even under a constrained parameterization 820 for ALT and temperature envelopes, accentuating the need for additional constraint(s) for a 821 better simulation of the freeze/thaw cycles.

822 Fig. 12H displays the envelopes of surface and thermal offsets (refer to Section 2.1 for definitions). The figure reveals high variability for the surface offset above the ground, 823 dominated by snow accumulation in winter and the shading effect of the canopy in summer. The 824 825 envelope of surface offset has positive values with a varying mean of 5° C-10°C and interannual 826 variability between of 2.2°C-5.5°C. Besides, the surface offset is the summation of winter and summer offsets, that when apportioned, highlights the significant influence of snow on keeping 827 permafrost from losing heat in winter over the impact of canopy shading in summer. Winter 828 offset could vary by up to ~10°C with an enormous interannual variability similar to that of 829 830 MAGTp (Fig. 12B), while summer offset has a weaker variance of ~5°C and a smaller 831 interannual variability, as shown in **Fig. A4**. On the other hand, the thermal offset, occurring in the soil above the permafrost's horizon, displays a confined uncertainty in order of 0.1°C-1°C, 832

noting that the thermal properties of soil texture above the permafrost table do exert the primary
influence on the thermal offset and JMC is characterized by the presence of organic soil –
ORGM*i* was well-identified according to the identifiability analysis for the JMC site based on
MAE (Fig. 11C).





840 Depth to the Zero Annual Amplitude (DZAA), E) BIAS of simulated ALT, F) MAE of simulated ALT,

- G) Date of Maximum thawing, and H) Surface and Thermal Offset. All presented variables correspond to
 the identifiable JMC experiments via the MAE (13 parameter set); refer to Fig. 2 for a brief description of
 permafrost variables; shading denotes the range of uncertainty, while red marks denote the available
- observation; each solid line in subplot G corresponds to a single model evaluation (parameter set).

845 Fig. 13 compares three different simulated temperature profiles for 1993, 1997, and 2000 at the JMC site for the behavioural parameter sets filtered by the MAE. The year 1993 (Fig. 12 and 846 Fig. 13A) has sound results for the ALT, DZAA, Tmax, and thermal offset at the cost of having 847 848 warmer permafrost (overestimated MAGTp and Tmin by ~1°C), shallower permafrost thickness (underestimated PB by 2m), and highly divergent surface offset. On the other hand, the year 849 850 1997 (Fig. 12 and Fig. 13B) gives good agreement for ALT, MAGTP, PB, DZAA, and a smaller 851 uncertainty range for the maximum thaw date in exchange for the highest observed underestimation of Tmin by 2°C in addition to a considerable variation of surface offset by 5°C. 852 Lastly, the year 2000 (Fig. 12 and Fig. 13C) has balanced results for ALT, DZAA, Tmin, and 853 854 Tmax, producing warmer (MAGTp overestimated by 1.2° C) and shallower permafrost thickness (PB underestimated by 2m) in addition to the immersive variability for the date of maximum 855 thaw (DOY130-DOY290). Such comparison highlights the difficulty/complexity that modellers 856 857 encounter while employing LSMs for permafrost-based applications, either investigative or predictive, regardless of the assessment scale. 858



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Fig. 13. The observed and simulated envelopes of temperature profiles (Tmin and Tmax) at the JMC site
 using identifiable parameters for MAE criteria at A) 1993, B) 1996, and C) 2000.

862 4 Summary and conclusions

Following extensive efforts to improve the realism of process representation in land surface 863 864 models (LSMs), their complexity and dimensionality has increased remarkably, complicating model/parameter identification. Moreover, simulating the dynamics of perennially frozen soil, or 865 permafrost, is further challenged by the significant thermal/hydraulic memories of a deep soil 866 column and the limited availability of ground observations. We note that the simulation of the 867 thermal regime dynamics of the soil column in cold regions directly influences the partitioning of 868 water and energy fluxes, which, if not well constrained, could yield deceptive future projections 869 870 for climate and hydrology. We inspected three interrelated issues regarding permafrost simulation in the MESH-CLASS LSM; the impact of input uncertainty (forcing data), the 871 872 sensitivity of simulations to model parameters, and the identifiability of model parameters. Three experimental sites within the Canadian Mackenzie River Basin (MRB) were employed in the 873 874 current study, characterized by various climatic conditions and permafrost zonation. We finally assessed model performance at one of the sites using a large set of permafrost characteristics 875 876 versus observations as available.

877 The combined impact of climate forcing and parameter uncertainty on permafrost dynamics was assessed for various climate forcing data sets, characterized by different temporal/spatial 878 879 resolutions and forecasting/reanalysis methods. Such characteristics can play a pivotal role in 880 initializing model states, parameter/model identification/sensitivities, and the subsequent 881 simulation quality. Three meteorological datasets were considered for the study; WFDEI, 882 WFDEI-GEM-CaPA, and WFDE5. Comparing the three forcing datasets to ground stations 883 highlighted the significant uncertainties that could be introduced to permafrost simulation due to persistent bias in air temperature and precipitation. Besides, it underlined associated issues with 884 885 forcing datasets, such as a repeated climatology-based (WFDEI-CRU variant) precipitation when there are no data available, in addition to the noticeable warm bias of air temperature in the 886 887 WFDEI-GEM-CaPA dataset, which exceeded the adiabatic lapse late correction (noting that 888 dataset provided data at 40m altitude).

The cumulative frequency distributions (CDF) for the averaged BIAS and MAE of Tmin, Tmax, and ALT were utilized for evaluating the experiments. No single dataset could collectively provide satisfactory model simulations for the three characteristics at the three sites. For instance, WFDEI-GEM-CaPA can reproduce the observations for Tmin and ALT using the BIAS and MAE criteria at the three sites, except for ALT at BWC, where WFDEI slightly outperforms. Thereby, the WFDEI-GEM-CaPA dataset was nominated for forcing the models of the three sites, to avoid inconsistent results for parameter sensitivity and identifiability if different forcing sets were used for the different sites.

897 Different global sensitivity analysis (GSA) experiments were implemented using the variogrambased framework (VARS) to study the degree of sensitivity of permafrost variables to the 898 899 perturbation of the MESH-CLASS parameters. Understanding, diagnosing, and developing 900 models for permafrost simulation were the motives for such vital analysis, given the 901 unavailability of a comprehensive (formal) GSA in the context of land surface modelling of permafrost. The traditional metric-based time-aggregate GSA was employed for different aspects 902 of permafrost dynamics, noting that model crashes were handled by a model emulation-based 903 904 substitution technique. The experiments accentuated the dominant role of parameters (ratio of sensitivity $\geq 10\%$) that describe heat insulation at the vegetation-soil interface, such as ZSNL, 905 906 LNZO, and ORGM*i*, and those that control the runoff generation processes, such as SDEP, DD, 907 and XSLP. The ranking and contribution of these parameters vary among experiments based on the incorporated response surface variable of the GSA. Further, the study provides a list of the 908 909 highly sensitive parameters for different permafrost characteristics. Remarkably, the water 910 ponding-related parameters possess a limited-to-negligible influence for all GSA experiments. 911 The study highlights model parameters that should be carefully fine-tuned and those with 912 negligible impact on output variability that, if fixed (e.g. to the median of parameter range) and 913 excluded from any subsequent model calibration, could reduce model dimensionality, the 914 associated computational cost, and enhance parameter identification.

Parameter identifiability was also investigated in a multi-objective fashion to examine model parameterization and fidelity with a different lens, complimentary to sensitivity and uncertainty analyses. An approach incorporating additional constraints on permafrost simulations and tight behavioural thresholds (based on a predefined measure of model performance) yielded a small number of parameter sets that satisfy the multi-objective criteria (*i.e.* 7-89 out of 26,200 sets). The analysis underscored that not all highly and moderately (10%> ratio of sensitivity \geq 1%) sensitive parameters were clearly identifiable among all experiments. Besides, the identifiable value/range for sensitive parameters differs among sites, highlighting the massive impact ofexternal forcing and predefined parameter ranges.

Permafrost dynamics, represented by various facets, were extensively examined for one of the 924 experiments (*i.e.* the MAE-based JMC experiment) to explore the uncertainty corresponding to 925 926 these designated behavioural solutions. Even though ALT, Tmin, and Tmax are mainly 927 replicated by the behavioural parameter sets with significant interannual variability, other descriptive factors of permafrost dynamics were not appropriately reproduced, such as MAGTp, 928 929 PB, the date of maximum thaw and the surface offset. Further, a qualitative comparison of the 930 simulated temperature profiles (at different years) and other permafrost variables highlighted the 931 challenges that modellers encounter while configuring LSMs for permafrost-related applications.

932 Despite the fact that the outcomes of this study were specific to the MESH-CLASS model and 933 limited to the selected evaluation sites and methods, they are practically beneficial for advancing 934 modelling practices, especially permafrost-related applications. The study highlighted the 935 complexities and challenges of LSM application in cold regions and shed light upon the possible approaches to address such obstacles. That being said, a joint multi-objective GSA and multi-936 objective identifiability analyses promote an improved understanding of LSM structure, reduces 937 predictive uncertainties, and facilitates efficient model calibration. Further, there is a pressing 938 need to develop improved forcing datasets that rectify the problems of the current versions of 939 datasets in terms of systematic biases and lack of interannual variability in air temperature and 940 941 precipitation for some datasets; other meteorological variables were not assessed due to data availability constraints. Besides, additional improvement is required in the MESH-CLASS model 942 to enhance the realism of permafrost simulation, as reflected by the simulation's 943 quality/uncertainty, e.g. producing cooler Tmin and misrepresenting surface/thermal offsets, 944 945 possibly due to insufficient insulation. Proposed modifications include the snow component which is still simulated via a single layer and the surface canopies where no explicit treatment of 946 947 canopy litter and moss is available. Lastly, future studies could be directed towards generalizing the outcomes of these analyses to other observational sites with more data and to other regions, 948 949 as well as exploring the extendibility of the work to various regional and global models with 950 varying complexity in large-scale applications.

951 Acknowledgement

952 This research was supported financially by the Canada Excellence Research Chair (CERC)

953 Programme in Water Security, Integrated Modelling Program for Canada (IMPC) and Razavi's

954 Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery Grant. The

955 authors would like to thank the Information & Communications Technology (ICT) at the

956 University of Saskatchewan, for providing continuous support in using the High-Performance

957 Computing (HPC) research cluster, Plato and Copernicus.

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1287 Appendix

1288 **Table A1.** Soil profile layering scheme for the two sites, adopted form (Elshamy et al., 2020).

Layer	Thickness	Layer	Thickness
1	0.1	14	1.48
2	0.1	15	1.78
3	0.11	16	2.11
4	0.13	17	2.48
5	0.16	18	2.88
6	0.21	19	3.33
7	0.28	20	3.81
8	0.37	21	4.34
9	0.48	22	4.9
10	0.63	23	5.51
11	0.8	24	6.17
12	0.99	25	6.87
13	1.22		



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Fig. A1. Same as Fig. 6, but showing the BIAS in maximum annual temperature envelope (Tmax).

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Fig. A2. Ratio of reliability of IVARS₅₀ for each parameter in all experiments for A) BIAS[Tmin], B) MAE[Tmin], C) BIAS[Tmax], D) MAE[Tmax], E) BIAS[ALT], and F) MAE[ALT].

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Fig. A3. Total ratio of sensitivity (based on IVARS₅₀) for each group of parameters (as indicated in Table
 2) for the MAE across all experiments.



Fig. A4. Temporal evolution and the associated range of uncertainty for A) Winter offset by accumulatedsnow, and B) Summer offset by the canopy's shading; gray shading denotes the range of uncertainty.