Evaluating Simplifications of Subsurface Process Representations for Field-scale Permafrost Hydrology Models

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6 Abstract. Permafrost degradation within a warming climate poses a significant environmental 7 threat through both the permafrost carbon feedback and damage to human communities and 8 infrastructure. Understanding this threat relies on better understanding and numerical representation of thermo-hydrological permafrost processes, and the subsequent accurate 9 10 prediction of permafrost dynamics. All models include simplified assumptions, implying a tradeoff 11 between model complexity and prediction accuracy. The main purpose of this work is to 12 investigate this tradeoff when applying the following commonly made assumptions: (1) assuming 13 equal density of ice and liquid water in frozen soil; (2) neglecting the effect of cryosuction in unsaturated freezing soil; and (3) neglecting advective heat transport during soil freezing and thaw. 14 15 This study designed a set of 62 numerical experiments using the Advanced Terrestrial Simulator 16 (ATS v1.2) to evaluate the effects of these choices on permafrost hydrological outputs, including both integrated and pointwise quantities. Simulations were conducted under different climate 17 18 conditions and soil properties from three different sites in both column- and hillslope-scale 19 configurations. Results showed that amongst the three physical assumptions, soil cryosuction is 20 the most crucial yet commonly ignored process. Neglecting cryosuction, on average, can cause 10% 21 ~ 20% error in predicting evaporation, $50\% \sim 60\%$ error in discharge, $10\% \sim 30\%$ error in thaw 22 depth, and $10\% \sim 30\%$ error in soil temperature at 1 m beneath surface. The prediction error for 23 subsurface temperature and water saturation is more obvious at hillslope scales due to the presence 24 of lateral flux. By comparison, using equal ice-liquid density has a minor impact on most 25 hydrological variables metrics of interest, but significantly affects soil water saturation with an averaged $5\% \sim 15\%$ error. Neglecting advective heat transport presents the least error, 5% or even 26 27 much lower, in most variables metrics of interest for a large-scale general Arctic tundra system 28 without apparent influence caused by localized groundwater flow, and can decrease the simulation time at hillslope scales by $40\% \sim 80\%$. By challenging these commonly made assumptions, this 29

30 work provides permafrost hydrology scientists important context for <u>understanding the underlying</u>

31 physical processes, including allowing modelers to better choose the appropriate process

- 32 representation for a given modeling experiment.
- 33

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42 1 Introduction

43 Permafrost describes a state of ground which stays frozen continuously over multiple years, which 44 may cover an entire region (e.g., Arctic tundra) or occur in isolation (e.g., alpine top). From the 45 perspective of scope, permafrost occupies approximately 23.9% (22.79 million km²) of the 46 exposed land area of the northern hemisphere (Zhang et al., 2008), as well as alpine regions and 47 Antarctica in the southern hemisphere. Permafrost areas store a vast amount of organic carbon, of 48 which most is stored in perennially frozen soils (Hugelius et al., 2014). If the organic carbon is 49 exposed due to permafrost thaw, it is likely to decay with microbial activity, releasing greenhouse 50 gas to the atmosphere and exacerbating global warming. In Arctic tundra, permafrost also plays 51 an important role in maintaining water, habitat of wildlife, landscape, and infrastructure (Berteaux 52 et al., 2017; Dearborn et al., 2021; Hjort et al., 2018; Sugimoto et al., 2002). Permafrost 53 degradation may cause significant damage to the local ecosystem, reshape the surface and 54 subsurface hydrology, and eventually influence the global biosphere (Cheng and Wu, 2007; 55 Jorgenson et al., 2001; Tesi et al., 2016; Walvoord and Kurylyk, 2016). Therefore, the occurrent 56 and potential impacts motivate the development of computational models with the goal of better 57 understanding the thermal and hydrological processes in permafrost regions, and consequently to 58 predict permafrost thaw more accurately.

59 Simulating soil freezing and thaw processes is a challenging task that incorporates mass and energy

60 transfer among atmosphere, snowpack, land surface (perhaps with free water), and a variably 61 saturated subsurface. Several hydrological models with different complexity and applicable scales 62 have been developed to investigate the complicated interactions. Reviews of permafrost models 63 based on empirical and physical representations using analytical and numerical solutions can be 64 found in (Bui et al., 2020; Dall'Amico et al., 2011; Grenier et al., 2018; Jan et al., 2020; Kurylyk 65 et al., 2014; Kurylyk and Watanabe, 2013; Riseborough et al., 2008). Process-rich models which aim to predict permafrost change through direct simulation of mass and energy transport, such as 66 the Advanced Terrestrial Simulator (ATS; Painter et al., 2016), GEOtop (Endrizzi et al., 2014), 67 68 CryoGrid 3 (Westermann et al., 2016), PFLOTRAN-ICE (Karra et al., 2014), and SUTRA-ICE 69 (McKenzie et al., 2007), have been demonstrated to describe thermal permafrost hydrology under various climate conditions. Nominally, representing more physical process complexity should 70 71 improve predictions of permafrost change, but the degree to which each process affects metrics of 72 permafrost hydrology is highly uncertain and likely differs by scale. Philosophically, models 73 provide a useful tool precisely because they allow counterfactual experiments where processes are 74 simplified to understand the relative importance of that process; thus, challenging assumptions 75 about process simplifications are a significant part of both general process understanding, benefiting the permafrost hydrology community writ large, and model representations, benefiting 76 77 the community of model developers and users.

Even in the most process-rich models of permafrost change, three such physical simplifications are often made: representing water at constant density (thereby neglecting the expansion of ice relative to liquid water), neglecting cryosuction of water in unsaturated, partially frozen soils, and neglecting advective heat transport.

82 First, because of the lower density of ice than liquid water, freezing water must expand the volume 83 of the porous media, push liquid water into nearby volume, or otherwise expand the volume 84 occupied by that water. As all-most of the current set of models operate under the assumption of a 85 rigid solid matrix and thus the absence of mechanical equations describing matrix deformation or 86 frost heave, including this expansion typically results in large pressures that must be offset by grain 87 compressibility or another mechanism. Therefore, the densities of ice and liquid water are 88 frequently assumed equal (e.g., Dall'Amico et al., 2011; Devoie and Craig, 2020; Weismüller et 89 al., 2011). It is uncertain whether this simplification affects predictions of permafrost change and 90 thermal hydrology.

91 Second, cryosuction describes the redistribution of water in partially frozen, unsaturated soils 92 caused by increased matric suction. At the interface of ice and liquid water, negative pressures 93 result in the migration of liquid water toward the freezing front and the subsequent increase of ice 94 content. Several approaches representing cryosuction in models are used (Dall'Amico et al., 2011; 95 Noh et al., 2012; Painter and Karra, 2014; Stuurop et al., 2021), either in an empirical form or 96 physically derived from the generalized Clapeyron equation. Other process-rich models have 97 ignored cryosuction entirely (McKenzie et al., 2007; Viterbo et al., 1999). Dall'Amico et al. (2011), 98 Painter (2011) and Painter and Karra (2014) evaluated their respective Clapeyron equation based 99 cryosuction models in soil column freezing simulations and presented a good match between 100 simulations and laboratory experiments in total water content (liquid and ice). Recently, Stuurop 101 et al. (2021) applied an empirical expression, a physics-based expression, and no cryosuction in 102 simulating soil column freezing process. They compared the simulated results with observations 103 from laboratory experiments. This comparison demonstrated minor differences between empirical 104 and Clapeyron-based cryosuction expressions, but the simulation without cryosuction cannot 105 predict the distribution of total water content in a laboratory-scale soil column. To our knowledge, 106 there is still no literature showing the effect of cryosuction on plot-scale permafrost predictions. 107 Third, heat transport in process-rich models is described using an energy conservation equation, 108 mainly including heat conduction, latent heat exchange, and heat advection. From a continuum-109 scale perspective, conductive heat transport is expressed in the form of a diffusive term based 110 on Fourier's law. Latent heat exchange accompanies phase change which alters the system enthalpy.

111 Advective heat transport describes the energy exchange caused by the flow of liquid water driven 112 by a hydraulic gradient (i.e., forced convection), which is expressed through an advective term in

energy balance equations. Additionally, other mechanisms that control heat transport, such as water vapor movement, thermal dispersion, etc., are neglected by nearly all models of permafrost

115 and are not considered here. Among these heat transport mechanisms, it is commonly recognized

116 that heat conduction predominates heat transport in the subsurface (Nixon, 1975). However, there

117 are also Several_studies have demonstrated the importance of advective heat transport in

118 permafrost hydrology through field observation analysis or modeling comparison. Such situations

119 where advective heat <u>transport</u> makes important contributions roughly fall into three categories.

120 The first centers on the development of taliks beneath lakes, ponds, topographic depressions, or

121 other discontinuous permafrost effects (e.g., Dagenais et al., 2020; Liu et al., 2022; Luethi et al.,

122 2017; McKenzie and Voss, 2013; Rowland et al., 2011). The second focuses on microtopographic 123 features that focus significant amount of water through small areas. This includes both low-center 124 ice wedge polygons associated with the formation of thermokarst ponds (e.g., Abolt et al., 2020; 125 Harp et al., 2021) and thermo-erosion gullies (e.g., Fortier et al., 2007; Godin et al., 2014). In these 126 cases, large, focused flows across small spatial scales allow advective heat transport to dominate. 127 The last category includes those studying the construction and maintenance of infrastructure 128 influenced by groundwater flow (e.g., Chen et al., 2020). Thus, these studies focus on either 129 location-specific or scale-limited problems. As McKenzie and Voss (2013) stated, whether heat 130 advection outweighs heat conduction depends on soil permeability, topography, and groundwater 131 availability. Relative to these special cases at small scales, we are more interested in to what extent 132 advective heat transport associated with liquid water flow contributes to permafrost hydrologic 133 change in a hillslope-scale or larger Arctic system. The Arctic systems, discussed hereinafter in 134 this paper, refer to those with negligible influence caused by localized groundwater flow features 135 as the three categories mentioned above. 136 To clarify the significant differences in model representations of permafrost, we investigate the

137 influence of including or not including these processes on permafrost change at plot-to-hillslope scales. We take the advantage of the flexibility offered by ATS to express multiple options of 138 139 process representation to implement this study in numerical experiments. For ice density, we 140 compare simulations with and without differences in ice density relative to water density; for 141 cryosuction, we compare simulations using a Clapyron equation-based expression and excluding 142 the cryosuction effect; and for heat transport, we compare simulations including or neglecting 143 advective heat transport. All comparisons are carried out across a range of Arctic climate 144 conditions and soil properties from three different sites. Both 1D soil-column-scale and 2D 145 hillslope-scale models are considered, in which varying hillslope geometries (i.e., 146 convergent/divergent hillslope) and aspects (i.e., north/south) are included. The aim of this study 147 is to provide permafrost hydrology modelers with crucial comparisons for better choosing a model 148 representation for a given study and better understanding permafrost physics by formally 149 considering the tradeoff between model complexity, accuracy, and, at least for one code, 150 performance. The aim of this study is to provide better understanding of physical processes to 151 permafrost hydrologists in general; and to offer some concrete insights to the model users and 152 developers working on the process-rich models with similar theories and equation basis.

153 2 Theory

154 The Advanced Terrestrial Simulator (ATS v1.2) (Coon et al., 2020) configured in permafrost mode 155 (Jan et al., 2018, 2020; Painter et al., 2016) was used to implement all numerical experiments in 156 this study. ATS is a process-rich code developed for simulating integrated surface and subsurface 157 hydrological processes, specifically capable of permafrost applications. It has been shown to 158 successfully compare to observations of seasonal soil freezing and thaw processes at different 159 scales. This includes 1D models of vertical energy transport typical of large-scale flatter regions 160 (Atchley et al., 2015), and 2D models admitting lateral flow and transport in Arctic fens (Sjöberg 161 et al., 2016), and polygonal ground (Jan et al., 2020).

162 The permafrost configuration of ATS comprises coupled water flow and energy transfer within 163 variably saturated soils and at land surfaces, a surface energy balance model describing thermal 164 processes in snow, and a snow distribution module for surface microtopography (Painter et al., 165 2016). The subsurface system solves a three-phase (liquid, ice, gas), two-component (water vapor, 166 air) Richards-type mass balance equation with Darcy's law and an advection-diffusion-conduction 167 energy balance equation. The surface system includes an overland flow model with diffusion wave 168 approximation, and an energy balance equation with an introduced temperature-dependent factor 169 describing the effect of surface water freezing. The subsurface system and surface system are 170 coupled through the continuity of pressure, temperature, and the corresponding fluxes by 171 incorporating the surface equations as boundary conditions of the subsurface equations (Coon et 172 al., 2020). The evolution of a snowpack and its effect on the surface energy balance is described 173 using an energy balance approach based on a subgrid model concept that includes all major heat 174 fluxes at the land surface. For a more detailed description of the permafrost configuration and 175 implementation in ATS, as well as key mathematical equations, the reader is referred to Painter et 176 al. (2016). Changes in this "most complex" model of permafrost hydrology are enabled by the 177 Arcos multiphysics library leveraged in ATS; this allows the precise model physics to be specified 178 and configured at runtime through the use of a dependency graph describing swappable 179 components in the model physics (Coon et al., 2016).

2.1 Ice density

181 The density of ice (kg/m³) is represented as a Taylor series expansion in both temperature and 182 pressure:

183
$$\rho_{i} = [a + (b + c\Delta T) \times \Delta T] \times (1 + \alpha \Delta p)$$
(1)

184 and the density of liquid water (kg/m^3) is represented as:

185
$$\rho_{l} = [a + (b + (c + d\Delta T) \times \Delta T) \times \Delta T] \times (1 + \alpha \Delta p)$$
(2)

186 where $\Delta T = T - 273.15$, $\Delta p = p_1 - 1e5$, T and p_1 are temperature (K) and liquid pressure (>101325

187 Pa), respectively; and a, b, c, d, α are constant coefficients, listed in Table 1. Under conditions of

188 equal density, we assume $\rho_i = \rho_l$.

189

Table 1 Coefficients in density of ice and liquid

	а	b	С	d	α
$ ho_{ m i}$	916.724	-0.147143	-2.38e-4	_	1.0e-10
ρ_1	999.915	0.0416516	-1.01e-2	2.06e-4	5.0e-10

190 <u>2.2</u> Cryosuction

191 Several models are available in the literature describing the relationship between unfrozen water 192 content and temperature or matric suction (e.g., Ren et al., 2017; Stuurop et al., 2021), which is 193 also termed the soil freezing characteristic curve. These models are either associated with 194 temperature empirically or related to the soil water retention curve through the Clapeyron equation. 195 The latter approach normally incorporates the soil cryosuction process, while the former does not. 196 Painter and Karra (2014) proposed a physics-based constitutive model which relates the soil 197 unfrozen water content with the van Genuchten model (van Genuchten, 1980) relationship for 198 phase partitioning of water in frozen soils based on the Clapeyron equation and Van Genuchten 199 model (Van Genuchten, 1980): $(S(P_0, I_{-9}), Q_{-1}, Q_{-1})$

200
$$s_{l} = \begin{cases} S_{*}(-\beta\rho_{l}L_{f}\vartheta), \vartheta < \vartheta_{f} \\ S_{*}(p_{g}-p_{l}), \vartheta \ge \vartheta_{f} \end{cases}, \ \vartheta = \frac{T(K)-273.15}{273.15}, \ \vartheta_{f} = -\frac{\psi_{*}(1-s_{g})}{\beta L_{f}\rho_{l}} \\ s_{i} = 1 - s_{l}/S_{*}(p_{g}-p_{l}) \end{cases}$$
(3)

where s_n is the saturation of *n*-phase and the subscripts n = 1, i, g are liquid, ice, and gas phases, respectively; β is a coefficient; L_f is the heat fusion of ice; p_n (n = 1, g) is the pressure of *n*-phase; S_* is the Van Genuchten model. This physically derived formulation can describe the change of matric suction in the frozen zone due to the change of ice content, and thus has the capacity to represent cryosuction. Alternatively, the unfrozen water content can be also expressed as a single-variable function

207 dependent on sub-freezing temperature for a given soil, ignoring the effect of cryosuction, such as

<u>dependent on sub-neezing temperature for a given son, ignoring the effect of eryosaetion, such as</u>

208 the following (McKenzie et al., 2007):to exclude the effect of cryosuction in this study, we used

209 the Van Genuchten model to determine the total water content, including liquid water and ice. The

210 liquid water content is achieved by an empirical relationship (soil-freezing characteristic curve)

- 211 which describes that the liquid water content only relates to temperature through an exponent
- 212 function (McKenzie et al., 2007).

213
$$s_{l} = s_{r} + (s_{sat} - s_{r}) \exp\left[-\left(\frac{T(K) - 273.15}{\omega}\right)^{2}\right]$$

$$s_{i} = S_{*}(p_{g} - p_{l}) - s_{l}$$
(4)

- 214 where s_r , s_{sat} are saturations of liquid water at residual and saturated conditions, respectively; ω is
- 215 a constant coefficient. In this case, the van Genuchten model was used to determine the total water
- 216 content, including liquid water and ice.

217 2.22.3 Advective heat transport

218 The energy conservation equation of the subsurface system is given by:

219
$$\frac{\partial}{\partial t} \left[\phi \sum_{n=l,i,g} (\rho_n s_n u_n) + (1-\phi) c_{v,\text{soil}} T \right] + \underbrace{\nabla \cdot (\rho_l h_l \mathbf{V}_l)}_{\text{advective heat}} \underbrace{-\nabla \cdot (\kappa_e \nabla T)}_{\text{conductive heat}} = Q_E$$
(5)

where ϕ is porosity; u_n is the specific internal energy of phase ($n \in \{1, i, g\}$); $c_{v,soil}$ (J m⁻³ K⁻¹) is the volumetric heat capacity of the soil grains. The second and third terms represent the advective and conductive heat transport in <u>the</u> subsurface, in which h_1 (J/mol) is the specific enthalpy of liquid; V_1 (m/s) is the velocity vector of liquid water determined by Darcy's law; and κ_e (W m⁻¹ K⁻¹) is the effective thermal conductivity of the bulk material including soil, air, liquid water, and ice. Q_E is the sum of all thermal energy sources (W/m³).

226 Similarly, the energy balance equation of the surface system is:

227
$$\frac{\partial}{\partial t} \{ [\chi \rho_{l} u_{l} + (1 - \chi) \rho_{i} u_{i}] \delta_{w} \} + \underbrace{\nabla \cdot (h_{l} \chi \rho_{l} \delta_{w} \mathbf{U}_{w})}_{\text{advective heat}} \underbrace{-\nabla \cdot \{ [\chi \kappa_{l} + (1 - \chi) \kappa_{i}] \delta_{w} \nabla T \}}_{\text{conductive heat}} = Q_{\text{net}}$$
(6)

228 in which χ is the unfrozen fraction <u>of surface</u> determined by surface temperature; δ_w is ponded 229 depth (m); U_w (m/s) is the velocity vector of liquid water on the surface determined by the 230 diffusion-wave approximated St. Venant equations (Gottardi and Venutelli, 1993) and Manning equation (Wasantha Lal, 1998); κ_n (W m⁻¹ K⁻¹) is the thermal conductivity of *n*-phase (*n* = 1, i); 231 232 $Q_{\rm net}$ (W/m³) is the net thermal energy into and out of ground surface, including that from solar 233 radiation, rain and snow melt, water loss by evaporation and to the subsurface, and conductive and advected heat transport to/from the subsurface. The second and third terms represent the (lateral) 234 advective and conductive heat transport that occur across the land surface. 235

236 3 Methods

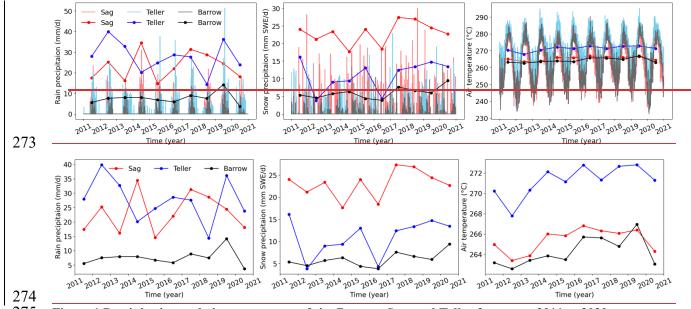
237 To evaluate the impact of representation of ice density, cryosuction, and advective heat transport 238 in permafrost modeling under different climate conditions and soil properties, we selected three 239 sites for their variance in climactic condition: Utqiagvik (Barrow Environmental Observatory, 240 71.3225° N, 156.6231° W), the headwaters of the Sagavanirktok (Sag) River (68.251° N, 149.092° 241 W), and the Teller Road Mile Marker 27 site on the Seward Peninsula (64.73° N, 165.95° W) in 242 Alaska. The simulated hydrological outputs for each site are compared in both column and 243 hillslope scenarios. Column scenarios represent expansive flat regions typical of the Arctic coastal 244 plains dominated by vertical infiltration and heat transport, and hillslope scenarios are 245 representative of the headwater, hilly terrain typical of the more inland permafrost.

246 In hillslope scenarios, hillslopes with northern and southern aspects are considered to investigate 247 physics representation comparisons under the same climate and soil condition (i.e., at a given site) 248 but different solar radiation incidence. Furthermore, hillslopes with both convergent and divergent 249 geometries are included to compare the sensitivity of simulated discharge on process 250 representation. These scenarios can incorporate many types of Arctic systems at the described plot-251 to-regional scales, but explicitly ignore the effects of microtopography or other local-scale 252 focusing mechanisms such as water tracts or thermo-erosion gullies. The objective is to reach a 253 conclusion on the influence of the three physics representations that can be widely applicable in 254 many Arctic systems.

255 **3.1 Field data description**

For each site, data used in each simulation comprises meteorological forcing datasets for the period
2011-2020, averaged wind speed, and soil properties.

258 Meterological forcing datasets are taken from the Daymet version 4 dataset (Thornton et al., 2020), 259 which provides observation-based, daily averaged weather variables through statistical modeling 260 techniques at 1 km spatial resolution (Thornton et al., 2021). Variables that are used in simulations 261 include daily average air temperature (calculated as the mean of Daymet's daily minimum and 262 maximum values), relative humidity (calculated from air temperature and Daymet's vapor pressure), incoming shortwave radiation (W/m²) (calculated as a product of Daymet's daylit 263 264 incoming radiation and daylength), and total precipitation (m/s), which is split into snow and rain 265 based upon the air temperature. Figure 1 illustrates the precipitation of rain, snow, and air temperature in-at the three sites from 2011 to 2020, where the points represent the corresponding averaged values per year. In terms of the forcing conditions, the annual rainfall of the Sag and Teller sites range between 20 and 40 mm/d over the ten years, more than twice the rainfall typical of the Barrow site. In addition, Sag has a significantly larger amount of snow every year that is over double of that at the Teller site and almost five times larger compared to the Barrow site. For the air temperature, Sag and Barrow are similar and colder than Teller by 7-8 degrees. In general, the Barrow site is dry and cold, the Sag site is wet and cold, and the Teller site is wet and warm.



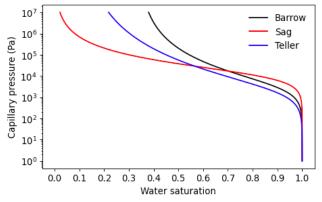
275 Figure 1 Precipitation and air temperature of site Barrow, Sag, and Teller from year 2011 to 2020

276 In addition to the time series of forcing data from Daymet, we used an average wind speed for each site. For Barrow and Teller, the average wind speed was estimated from the measurement 277 taken by the Next-Generation Ecosystem Experiments (NGEE) Arctic project. At Barrow, the 278 279 measurement was taken at area A (71.2815° N, 156.6108 ° W) at the height of 1.3 meters above 280 surface (Hinzman et al., 2014). At Teller, the measurement at 3.8 m above the surface of a lower 281 level of the watershed (Busey et al., 2017) was used. For Sag, the average wind speed was 282 estimated based on the measurement at the Toolik Lake field site (near to Sag River) at the height 283 of 3.1 m above surface, which is accessible through the National Ecological Observatory Network 284 (NEON, 2021).

The soil properties of Barrow, Sag, and Teller, including porosity, permeability, Van Genuchten parameters, and thermal conductivity parameters, were chosen from previous modeling studies at

these sites (Atchley et al., 2015; Jafarov et al., 2018; O'Connor et al., 2020), see (Table 2). Roughly,

the soil profile of each site is composed of two materials: the top organic-rich layer comprising mosses, peats, and other organic rich soils measuring approximately 10-30 cm thick, and the principal mineral soil. There is minor difference in thermal conductivity parameters among the three sites, and soil permeability is also at the same order of magnitude. The soil-water characteristic curve (SWCC) of the principal mineral soil of Barrow, Sag, and Teller, shown in Figure 2, indicates that the soil propert<u>iesy between at</u> Barrow and Teller <u>is are</u> relatively similar, while Sag differs from the other two with a relatively flat SWCC.



295 296 Figure 2 Soil-water characteristic curve (SWCC) of soil in Barrow, Sag, and Teller

297 Usually, at the hillslope scale, the thickness of organic layers of a watershed varies from the toe-298 slope, through a steeper mid-hill, up to the flat top. Typically, thicker organic layers may exist at 299 the top and bottom compared to the mid-hillslope. The low thermal conductivity of organic layers 300 can impede the heat transport between the air and the underlying mineral soil, resulting in varying 301 thaw depth (or permafrost table depth) along a hillslope, which has been observed at the site Teller (Jafarov et al., 2018). In this paper, hillslope meshes were constructed following this observation 302 303 so that the organic layers are thicker at the top and bottom of a hillslope, as described in the next 304 section.

305 3.2 Mesh design and material properties

The comparison of different physics representations was conducted in both column and hillslopescenarios.

The column model was designed as a one-dimensional, 50 m deep domain. The column domain was discretized into 78 cells with gradually increasing cell thickness, starting from 2 cm at the soil surface to 2 m at the bottom of the domain. We assigned different material properties to the cells to represent different soil layers. A column domain is divided into three layers, and the thickness of each layer was designed differently among the three sites according to geological observations (Jan et al., 2020; O'Connor et al., 2020; NGEE-Arctic). Specifically, from top to bottom, the three layers of the Barrow soil column are 2 cm-thick moss, 8 cm-thick peat, and mineral; for Teller, the soil column consists of a 4 cm moss layer, a 22 cm peat layer, and mineral; and the three layers of the Sag soil column are acrotelm, catotelm, with thickness of 10 cm and 14 cm, respectively, and the remainder mineral. The soil properties of each layer at three sites are listed in Table 2.

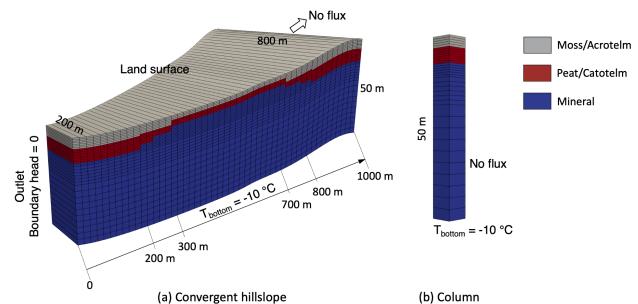
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Table 2 Soil properties of three soil layers of all sites used in this paper

Site		Barrow			Sag			Teller	
Layers	moss	peat	mineral	acrotelm	catotelm	mineral	moss	peat	mineral
Porosity	0.9	0.876	0.596	0.878	0.796	0.457	0.9	0.55	0.45
Permeability (m ²)	1.7e-11	9.38e-12	6e-13	2.64e-10	9.63e-12	3.98e-13	5e-11	5e-12	2e-13
VG α (Pa ⁻¹)	2.3e-3	9.5e-4	3.3e-4	7.93e-4	1.75e-4	8.06e-5	2.35e-3	2.93e-4	5.45e-4
VG n	1.38	1.44	1.33	1.405	1.566	1.571	1.38	1.269	1.236
Residual saturation	0.056	0.388	0.334	0.0073	0.0662	0.	0.1	0.	0.1
Thermal conductivity, unfrozen (Wm ⁻¹ K ⁻¹)	0.446	0.427	0.788	0.519	0.630	1.309	0.57	0.67	1
Thermal conductivity, dry (Wm ⁻¹ K ⁻¹)	0.024	0.025	0.104	0.066	0.086	0.265	0.07	0.07	0.29

319

320 In the hillslope scenario, we designed the mesh based on observations at Teller to represent a 321 generalized, varying-thickness low Arctic hillslope. A hillslope mesh was created first by 322 generating a pseudo-2D surface mesh with 50 cells and then extruding the 2D mesh downward by 323 50 m. The pseudo-2D surface was designed in a trapezoidal shape with a single, variable-width 324 cell in the cross-slope direction to represent convergent/divergent hillslopes, the short and long 325 sides of which are 200 m and 800 m, respectively (see Figure 3). Vertically, from surface 326 downward, the grid size distribution was the same as the column mesh for each site. The domain is also composed of three layers, same as the column, while the numbers of cells representing each 327 328 soil layer (i.e., soil layer thickness) are different along the hillslope. The thickness distribution of 329 the first two layers of each site is shown in Table 3. The third layer of a hillslope for all sites is the 330 principal mineral soil. Additionally, hillslope meshes with different aspects (i.e., north-facing, south-facing) were also created. 331



(a) Convergent hillslope
 (b) Column
 (c) Convergent hillslope
 (c) Column
 (c) Column</l

335

Table 3 Thickness distribution of the organic layers along hillslope for each site

Site	Horizontal <i>x</i> range (m)	Barrow layer thickness (cm)	Sag layer thickness (cm)	Teller layer thickness (cm)
	1000000000000000000000000000000000000	2	14	<u>8</u>
Layer 1 -	$300 \sim 700$	2	6	4
Moss/Acrotelm	$800 \sim 1000$	2	14	8
L avian 2	$0 \sim 200$	12	18	22
Layer 2 - Peat/Catotelm -	$300 \sim 700$	6	8	22
	$800 \sim 1000$	12	18	22

336 3.3 Model setup

337 To study how the representations of the three physical processes (i.e., ice expansion represented 338 by density, cryosuction, and advective heat transport) affect simulated hydrological outputs at different scales and hillslope topography features, and under various forcing and soil conditions, 339 340 62 model simulations were conducted, summarized in Table 4. To examine the validity of the 341 assumption of equal density between ice and liquid water, we included cryosuction and advective 342 heat transport in models. To investigate the role of cryosuction in permafrost modeling, we used 343 different density, while neglecting advective heat transport to decrease the computation cost. Note 344 that neglecting advective heat transport in these runs can reduce the effect of cryosuction on simulation predictions, as cryosuction moves water which would itself advect energy. To compare 345 346 the difference between neglecting and including heat advection, we used different density expressions for ice and liquid, and included cryosuction. Particularly, in order to understand the 347

348 impact of advective heat transport on permafrost processes when soil is at its wettest, we designed 349 two extreme cases under the warm, wet conditions of the Teller site in which soil evaporation was 350 factitiously artificially reduced. These runs were designed to maximize water flux and therefore 351 maximize the potential for advective heat transport to affect predictions.

To compare	Site	Scale	Geometry	Aspect	Remark
		column	_	_	_
• $\rho_i \neq \rho_l$, Eq. (1)	Barrow		convergent	north	 heat advection
	Sag	hillslope	convergent	south	
• $\rho_{\rm i} = \rho_{\rm l}, {\rm Eq.} (2)$	Teller	misiope	divergent	north	• cryosuction
			uivergent	south	
	-	column	_	_	_
 Include heat advection 	Barrow Sag Teller	hillslope	convergent -	north	• $ ho_{ m i} eq ho_{ m l}$
• Include heat advection			convergent	south	• cryosuction
• Neglect heat advection		misiope	divergent -	north	
• Neglect heat advection			uivergent	south	
	Extreme case, Teller	hillslope	convergent	north	 reduced evaporation
	<u> </u>	column	_	-	_
 Include cryosuction 	Barrow		convergent	north	• $\rho_{\rm i} \neq \rho_{\rm l}$
	Sag	hillslope	convergent	south	• no heat advection
 Neglect cryosuction 	Teller	misiope	divergent	north	
			uvergent	south	

Table 4 Ensemble of models designed in this study

353

352

354 Prior to simulating all cases, two steps of initialization are carried out for each site. First, a column 355 model initially above freezing temperature with a given initial water table depth and above-0 °C 356 temperature was frozen by setting the bottom temperature at a constant value of -10 °C until a 357 steady-state frozen soil column is formed. The initial water table depth is chosen to ensure that the 358 frozen column's water table, after accounting for expansion of ice, is just below the soil surface. 359 The pressure and temperature profiles of the frozen column were used as the initial conditions of 360 the second step initialization. Before proceeding, the observed forcing data (period of 2011-2020) 361 was averaged across the years to form a one-year, "typical" forcing year, which was then repeated 362 10 times. Using this typical forcing data and the solutions of the first step, we solved the column model in a transient solution, calculating an annual cyclic steady state and obtaining the pressure 363 364 and temperature fields at the end of the 10th year. The final pressure and temperature profile of the 365 column at the end of the 10-year simulation state was then assigned to each column of the hillslope 366 mesh used as the initial condition in the formal simulations listed in Table 4. The temperature at the bottom was constant at -10 °C. 367

368 **3.4 Evaluation metrics**

369 To fully assess the effect of representation of ice density, advective heat transport, and cryosuction

- 370 in permafrost hydrology modeling, we used <u>the</u> root mean squared error (RMSE) and normalized
- 371 Nash–Sutcliffe efficiency (NNSE) as performance metrics. RMSE has the same dimension as the
- 372 corresponding variables, which can be used to evaluate the average absolute deviation from a
- 373 benchmark, defined by:

374 RMSE =
$$\sqrt{\frac{\sum_{t=1}^{N} (x_t - y_t)^2}{N}}$$
 (7)

where x_t and y_t are the two modeled datasets to compare from the initial time point (t = 1) to the end (t = N).

NNSE is a normalized dimensionless metric describing the relative relationship between an
estimation and a reference, which is oftentimes used for evaluating hydrological models¹/₂-

379 NNSE =
$$1/\left(1 + \frac{\sum_{t=1}^{N} (x_t - y_t)^2}{\sum_{t=1}^{N} (x_t - \bar{x})^2}\right)$$
 (8)

380 where the modeled results x_t (obtained without physics simplification) are considered as the 381 benchmark, and \bar{x} is the mean value of the benchmark. A NNSE approaching 1 indicates perfect 382 correspondence between two groups of values in comparison-observations.

In addition, we also used <u>the normalized mean absolute error (MAE)</u> to quantify the percentage
change of results obtained with simplified physics relative to full physical representations (see
Section 4.4):-

386 Normalized MAE =
$$\frac{\sqrt{\sum_{t=1}^{N} |x_t - y_t|/N}}{\text{normalizing reference}} \times 100\%$$
 (9)

387 Two normalizing references were selected considering different <u>modeled metrics of interestmodel</u>
 388 output variables. For instance, in terms of temperature and saturation which fluctuate between two

389 non-zero values, the annually averaged variation range was chosen as the reference:-

390 Normalizing reference =
$$\frac{\sum_{y \in ar=1}^{num \text{ of } y \in ars}(\text{maximum -minimum})}{\text{number of } y \in ars}$$

391 For variables a modeled metric with zero as the smallest value, such as evaporation, discharge,

392 and thaw depth, the corresponding average value was selected as the reference.

393 4 Results

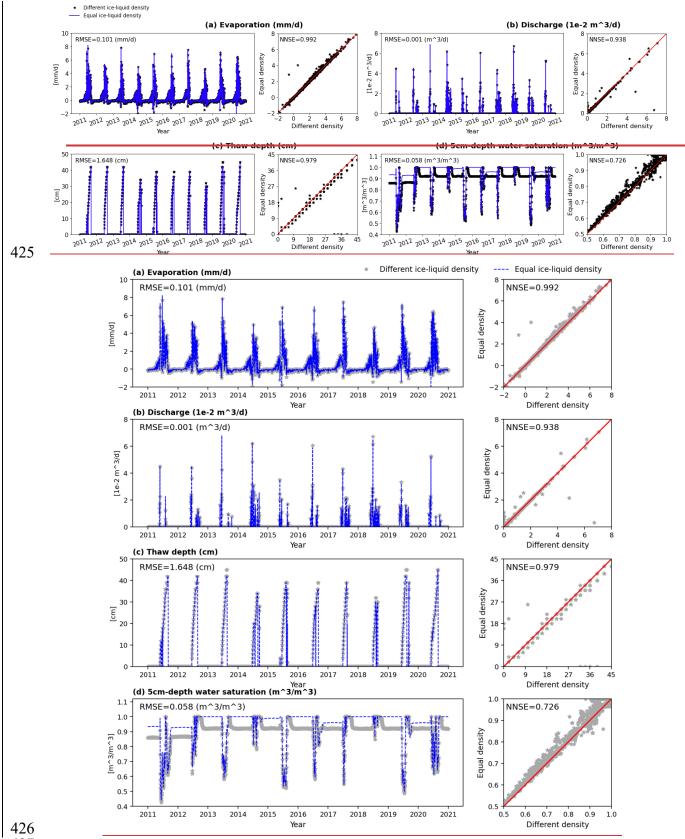
394 This section compares simulated outputs over the period of 2011-2020 for the three physicals

395 <u>processes</u> under different simulating conditions. We focus on the impact on integrated 396 <u>variablesmetrics</u>, such as evaporation, discharge, averaged thaw depth, and depth-dependent 397 <u>variablesmetrics</u>, such as temperature, and total water saturation (ice and liquid). For hillslope 398 models, we chose five surface locations according to the slope geometry to collect simulated data, 399 which were then averaged to obtain a single outcome for each <u>variable-metric</u> of interest.

400 **4.1 Ice density**

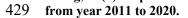
401 To evaluate the representation of ice density on permafrost process simulation, we compared 402 evaporation, discharge, thaw depth, and total water saturation between simulations using equal and 403 different ice density expressions. Figure 4 and Figure 5 show an example of the comparison under 404 conditions of Sag at column and hillslope scale<u>s</u>, respectively. Results are compared in both time 405 series and correlation.

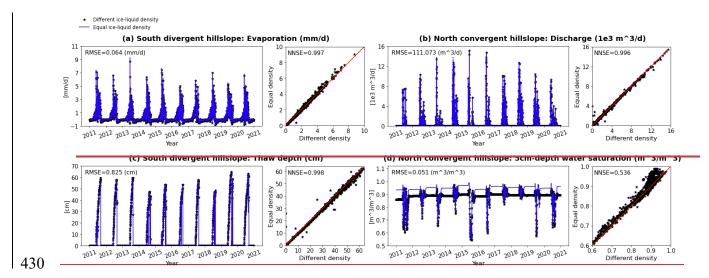
406 Generally, at both column and hillslope scales, assuming equal density between ice and liquid has 407 minor impacts on evaporation, discharge, and thaw depth over the 10-year simulation, except at a 408 few deviated points as shown in the correlation figures. According to column-based models, the 409 RMSEs of evaporation, discharge, and thaw depth are 0.101 mm/d, 0.001 m³/d, and 1.648 cm, 410 respectively, one order of magnitude smaller than the values of the corresponding variable metrics 411 values. At the hillslope scale (see Figure 5) the south-facing divergent hillslope is selected to show 412 modeling comparison on evaporation and thaw depth, in that they are potentially mostly affected 413 when a hillslope has a south orientation and divergent geometry. Likewise, the north-facing convergent hillslope is chosen to compare discharge and water saturation from simulations with 414 415 different density expressions. Even then, RMSEs of the three variables metrics are 0.064 mm/d, 416 111.073 m³/d, and 0.825 cm, respectively, two orders of magnitude smaller than the values of the 417 corresponding variable values metrics at the hillslope scale. Besides, NNSEs of the three variables 418 metrics output from both column and hillslope simulation are over 0.9, approaching 1 especially 419 at the hillslope scale. Therefore, all indicate good performance of equal ice-liquid density 420 assumption in predicting integrated variables metrics and thaw depth. By comparison, the 421 estimation of water saturation is relatively more affected by the density assumption during cold 422 seasons within a year, as shown by Figure 4 (d) and Figure 5 (d). This is reasonable in that when 423 water mainly exists in the form of ice, equal ice-liquid density assumption will overestimate the 424 water content.



427 Figure 4 Comparison of column simulations between different and equal ice-liquid density under conditions

428 of Sag, in (a) evaporation, (b) discharge, (c) thaw depth, and (d) water saturation at 5 cm beneath surface





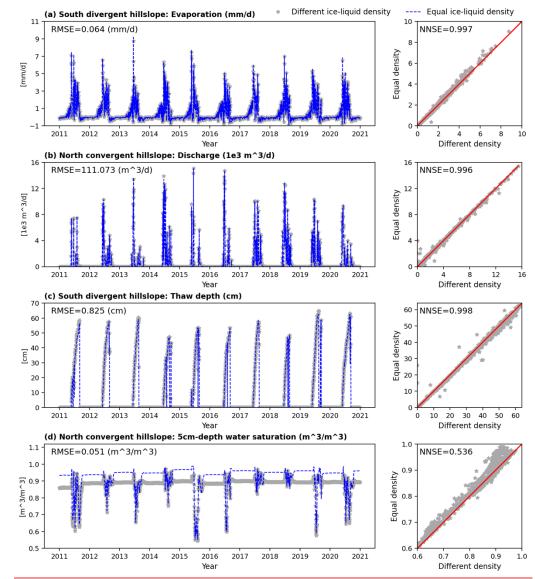
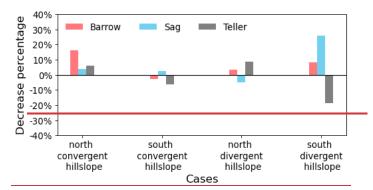




Figure 5 Comparison of hillslope simulations between using different and equal ice-liquid density under
conditions of Sag, in (a) evaporation, (b) discharge, (c) thaw depth, and (d) water saturation at 5 cm beneath
surface from year 2011 to 2020.

435 In addition, we investigated how much the assumption of equal ice-liquid density can affect 436 simulation time at hillslope scale. Using 10-year simulations with real ice density as references, the percentage change of time consumed after applying equal ice-liquid density was calculated and 437 displayed in Figure 6. Overall, under the density assumption, it may take less time (positive 438 percentage), but no more than 25% and on average lower than 10%. However, it may also increase 439 440 computational time (negative percentage) mainly under wet conditions, such as at Sag and Teller. 441 Thus, given a long-period large-scale modeling of permafrost freezing and thaw process, there is 442 no consistent conclusion on whether equal ice-liquid density can ease computational cost. It

443 depends on both the weather conditions and soil properties.

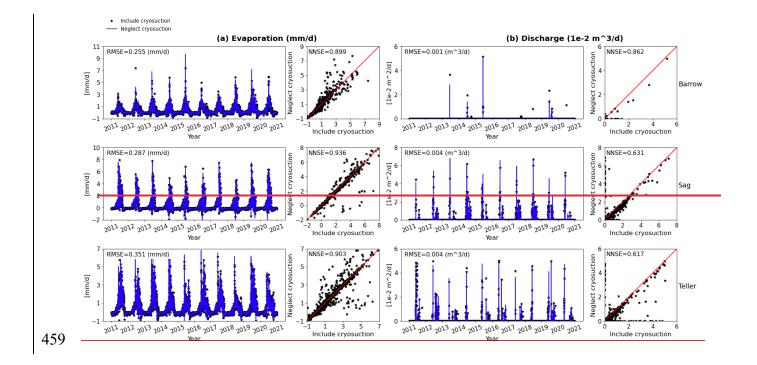


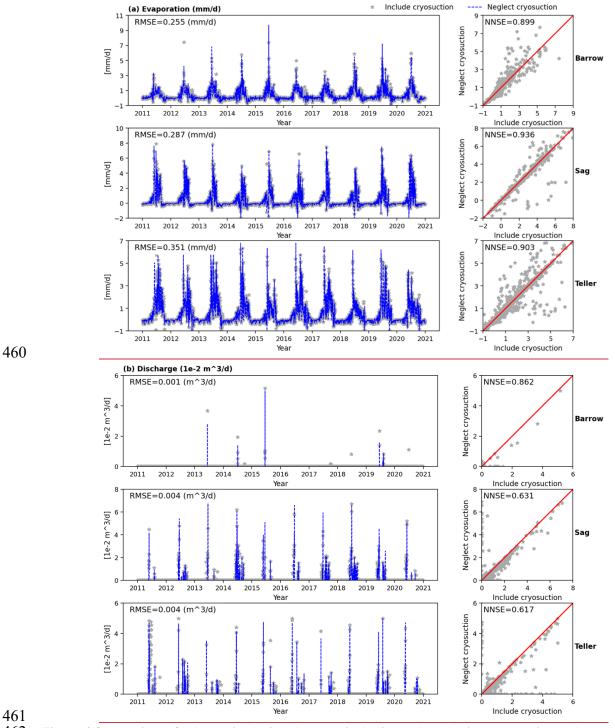
444 445

Figure 6 Decreased percentage of simulation time under the assumption of equal ice-liquid density compared
 to the real ice density representation for all hillslope scale simulations.

447 **4.2** Cryosuction

448 To evaluate the effect of cryosuction on permafrost process predictions, we compared evaporation, 449 discharge, thaw depth, total water saturation, and temperature obtained through simulations 450 including and neglecting cryosuction. Figure 6 through Figure 8 illustrate column-scale 451 comparisons of these variables metrics under conditions at the three sites (Barrow, Sag, and Teller). 452 Figure 6 presents the effect of excluding cryosuction on evaporation and discharge. The RMSE of evaporation from the three sites ranges between 0.25 mm/d and 0.35 mm/d, still one order of 453 454 magnitude smaller than the common evaporation rate. Evaporation NNSEs of the three sites are around 0.9. For discharge, RMSEs are also one order of magnitude smaller than the average, 455 whereas NNSEs fall between 0.6 and 0.9. Generally, cryosuction plays a more important role in 456 457 predicting discharge compared to evaporation, especially under warm and wet climate conditions, 458 such as Teller.



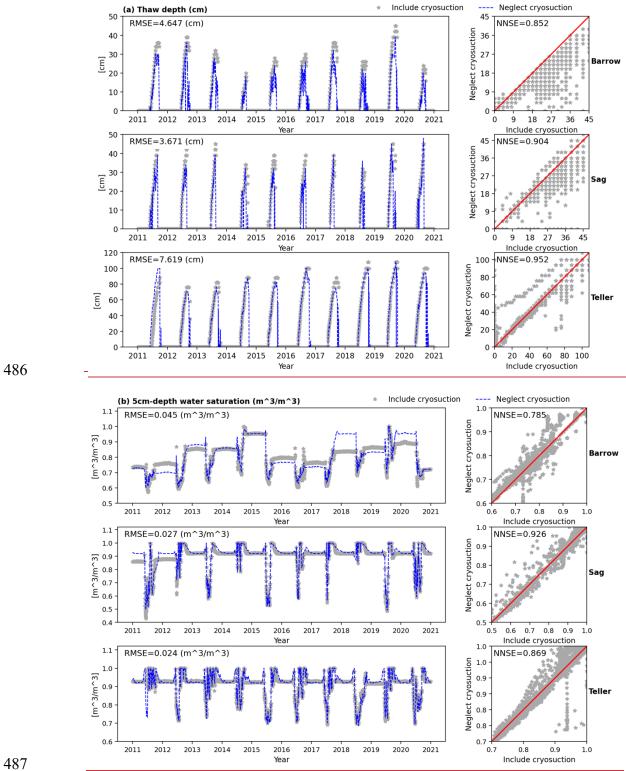


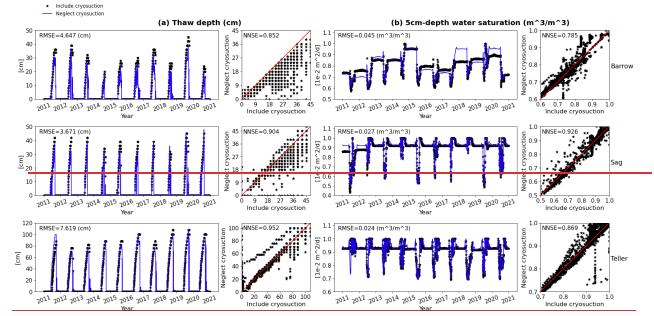
462 Figure 6 Comparison of column simulations between including and neglecting cryosuction under conditions
463 of Barrow, Sag, and Teller, in (a) evaporation, (b) discharge.

464 Figure 7 shows the effect of cryosuction on column-scale simulated thaw depth and total water
465 saturation at 5 cm beneath <u>the surface</u>. <u>Overall, neglecting cryosuction tends to underestimate the</u>

466 deepest thaw depth. As already mentioned, cryosuction, in essence, increases soil suction to attract

467 more liquid water moving towards the frozen front during soil freezing. Thus, the real active layer 468 formed due to the existence of cryosuction should be thicker than the cases in which cryosuction 469 is assumed unimportant. RMSEs of thaw depth in Figure 7 range from 3 cm to 8 cm. Though still 470 one order of magnitude smaller than the average annual thaw depth, the estimation error due to 471 neglecting cryosuction is most obvious in summer, especially at areas with cold temperature like 472 Barrow. RMSEs of thaw depth range from 3 cm to 8 cm. Though still one order of magnitude 473 smaller than the average annual thaw depth, the estimation error due to neglecting cryosuction is obvious in summer, especially at areas with cold temperature and low rainfall like Barrow. By 474 475 comparison, at Teller, where the largest thaw depth is over double that of Barrow and Sag due to 476 its higher temperature, soil cryosuction does not essentially affect thaw depth compared to the 477 other two sites. Similarly, for the total water saturation, at Barrow, the effect of cryosuction is 478 more clearly observed, not only during cold seasons as observed for density representation (section 479 4.1), but also in summers. The reason why Barrow is more sensitive to the cryosuction process on 480 predicting thaw depth and water content is determined by both soil properties and climate 481 conditions. The soil at Barrow has larger suction and is able to hold more water (see Figure 2), 482 providing the possibility for cryosuction to make contributions. Moreover, the principal difference 483 between cryosuction and non-cryosuction representations is presented when the temperature is 484 below the freezing point (see Eq.(3) and Eq.(4)). Compared to Sag and Teller, Barrow has lower 485 annual average temperature (see Figure 1), making the effect of cryosuction more pronounced.

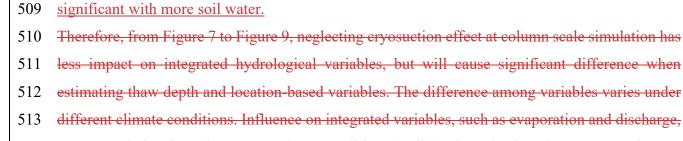




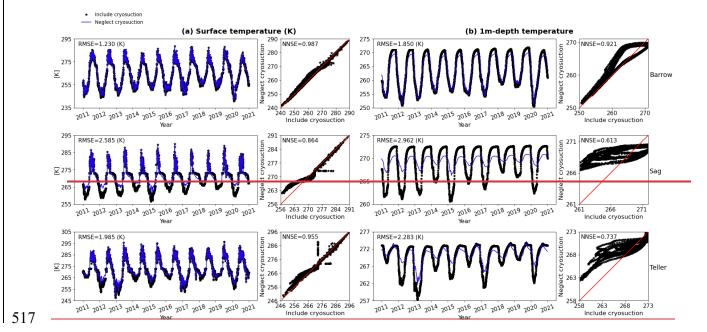
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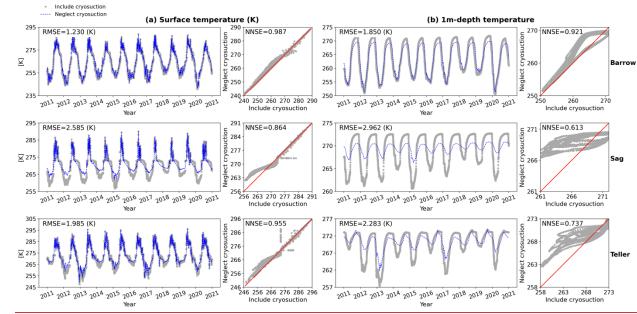
Figure 7 Comparison of column simulations between including and neglecting cryosuction under conditions
 of Barrow, Sag, and Teller, in (a) thaw depth, (b) water saturation at 5 cm beneath surface.

491 Finally, we also compared soil temperature obtained from models with or without cryosuction 492 included; in-see Figure 8. Surface temperature is little affected by cryosuction, except at the Sag 493 site, where the surface temperature is overestimated during winter. At 1 m depth, soil temperature 494 of Barrow is slightly changed in summer due to neglecting cryosuction. At both Sag and Teller, 495 the fluctuation range of temperature at 1 m beneath land surface is underestimated if the 496 cryosuction effect is not considered, especially at Sag, NNSE decreases to 0.6-approximately 0.6. 497 The reason that causes Sag and Teller are more sensitive to the effect of cryosuction on temperature 498 is associated with the larger water amount in the two sites. During freezing, soil freezes from 499 ground surface downward and from the bottom of active layer upward, forming a liquid zone in 500 between where the temperature approximates freezing point due to phase change (Figure S3.1(a) 501 in the Supplement shows an example of the column model under the Sag River condition at the 502 <u>300th day of one year). Thus, this liquid zone isolates the upper permafrost from the soil surface</u> 503 temperature variations due to the weakened conductive heat transport along the soil depth. 504 Additionally, the released latent heat in this liquid zone may retard soil freezing, which also tends 505 to reduce thermal conduction. However, cryosuction can speed up freezing and promote the 506 attenuation of the liquid zone (see S3.1(a) and (b) in Supplement. Figure S3.1(b) shows the 507 ice saturation at the same time with Figure S3.1(a), when the soil column still has large non-frozen area), and thus decrease the impact of the liquid zone. Hence, the influence of cryosuction is more 508



- 514 are more obviously under warm and wet conditions (Teller); thaw depth and water saturation are
- 515 affected more under cold and low-rainfall conditions (Barrow); and soil temperature tends to be
- 516 influenced greater under cold and high precipitation (rain and snow) conditions (Sag).





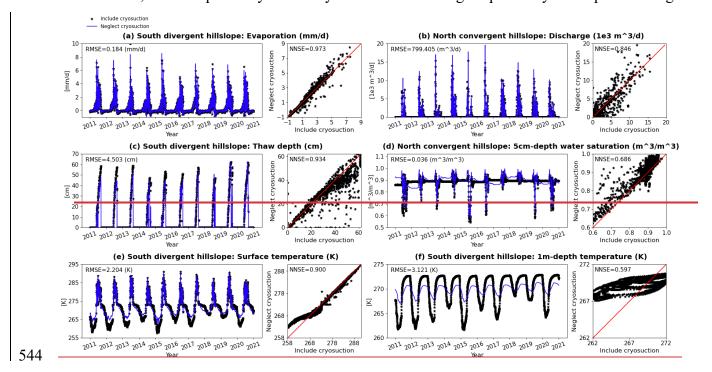
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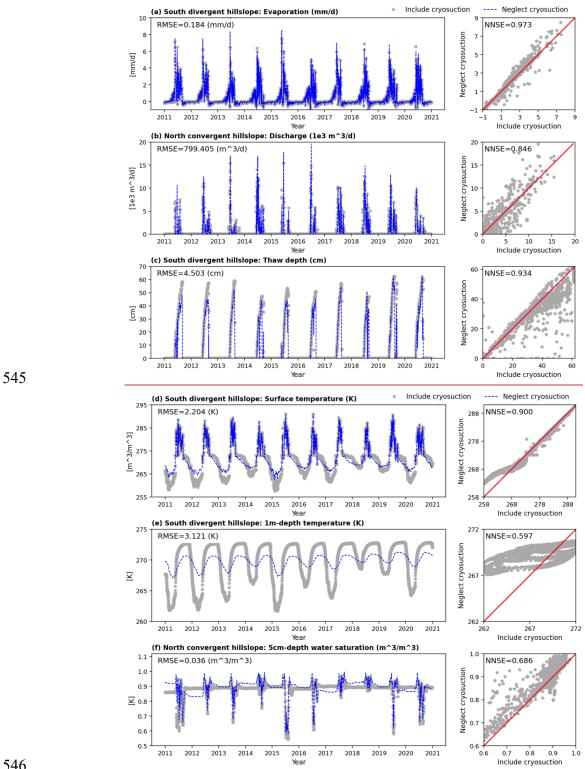
519 Figure 8 Comparison of column simulations between including and neglecting cryosuction under conditions 520 of Barrow, Sag, and Teller, in (a) surface temperature, (b) temperature at 1 m beneath surface.

521 Therefore, from Figure 6 to Figure 8, neglecting the cryosuction effect in column-scale simulations 522 has less impact on integrated hydrological metrics, but will cause significant difference when 523 estimating thaw depth and location-specific metrics. The difference among these metrics varies 524 under different climate conditions. Integrated metrics, such as evaporation and discharge, are 525 affected more under warm and wet conditions (Teller); thaw depth and water saturation are 526 affected more under cold and low-rainfall conditions (Barrow); and soil temperature tends to be affected more under cold and high precipitation (rain and snow) conditions (Sag). 527 528 Neglecting soil cryosuction has a similar impact on hydrological outputs in hillslope scale models.

529 Figure 9 shows the comparison of the variables-metrics of interest discussed above under the Sag 530 climate. Evaporation, thaw depth, and temperature are presented based on south-facing divergent 531 hillslope models, while discharge and water saturation are from hillslope models with north-facing convergent geometry. In general, neglecting soil cryosuction has a smaller effect on integrated 532 533 variables metrics (evaporation and discharge) compared with other pointwise variables metrics. 534 Though that depth presents a high NNSE of approximately 0.94, and low RMSE of about 4.5 535 cm compared to the average, indicating a good match between models considered and excluded cryosuction, the estimation error during summer may reach as high as 10 cm, particularly from 536 537 2011 to 2017, as shown in Figure 9 (c). Obvious errors in water saturation and temperature, similar with column-scale models, occur almost annually with respect to extrema during winter and 538

539 summer. Overall, compared to column-scale models, differences in evaporation, discharge, thaw 540 depth, and surface temperature due to neglecting cryosuction effect-are relatively reduced at <u>the</u> 541 hillslope scale if comparing NNSEs (Table 5). Localized subsurface <u>variablesmetrics</u>, such as 542 water saturation and 1m-depth soil temperature, show increased errors from column to hillslope 543 scale models, which is primarily caused by lateral flux exchange captured by hillslope modeling.







547 Figure 9 Comparison of hillslope simulations between including and neglecting cryosuction under conditions

548 of Sag, in (a) evaporation, (b) discharge, (c) thaw depth, (d) water saturation at 5 cm beneath surface, (e)

550 551

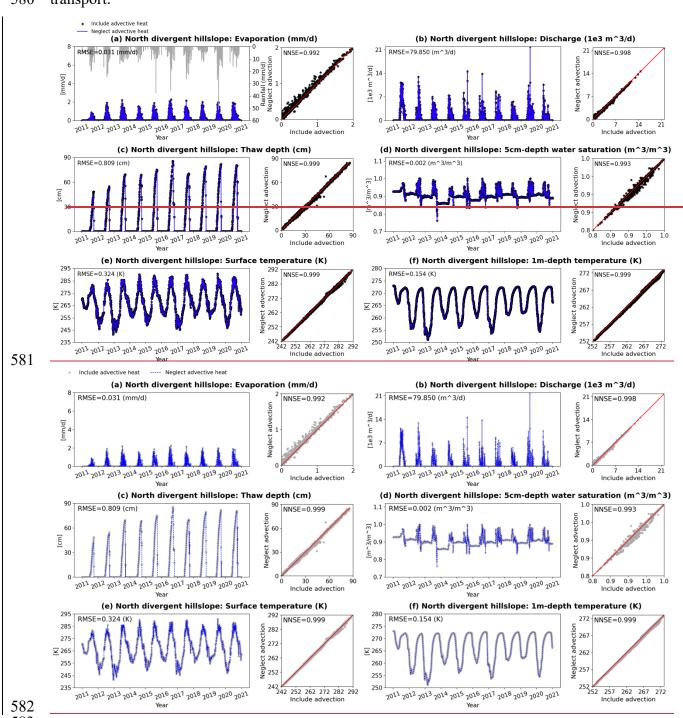
Table 5 NNSE of outputs from column and hillslope models under conditions of Sagshown in Figure 6 through Figure 9

Scale	Evaporation (mm/d)	Discharge (m ³ /d)	Thaw depth (cm)	5cm-depth water saturation (-)	Surface temperature (K)	1m-depth temperature (K)
Column	0.936	0.631	0.904	0.926	0.864	0.613
Hillslope	0.973	0.846	0.934	0.686	0.900	0.597

552

553 **4.3 Advective heat transport**

554 This section evaluates the performance of advective heat transport in modeling permafrost process. 555 As above, we investigated the influence of neglecting heat advection on evaporation, discharge, 556 thaw depth, total water saturation, and temperature. Overall, after comparing all hydrological 557 outputs from models with different heat transport representations, heat advection is proved 558 insignificant does not play a vital role in an normal Arctic system where the influence of localized 559 groundwater flow can be neglected. after comparing all hydrological outputs from models with 560 different heat transport representations. Comparisons based on column-scale and hillslope-scale 561 models are not shown here (see Supplement); instead, the extreme case under conditions of Teller 562 is presented (Figure 10). Teller is abundant in rainfall over the period of 2011-2020 (Figure 1). In 563 the extreme case, evaporation was reduced factitiously artificially to almost a quarter of the original 564 value (see Figure 6 (a) at Teller and Figure 10 (a)) for the purpose of increasing water flow rates. 565 For instance, discharge has quadrupled after adjusting evaporation by comparing Figure 10 (b) and 566 Figure 6 (b) at Teller. This specific scenario is chosen to maximize the potential effect of advective 567 heat transport in a hillslope-scale Arctic system. Figure 10 illustrates comparisons on all outputs 568 mentioned above from hillslope models without heat advection and with full thermal 569 representation. Apparently, all RMSEs are extremely small, at least two orders of magnitude lower 570 than the corresponding variable-metric average. Almost all NNSEs are approximately one, even 571 for thaw depth, localized water saturation, and temperature. Under the assumption of large-scale 572 Arctic systems ignoring the influence by localized groundwater flow features (e.g., ponds, gullies, 573 etc.), the liquid water flux determines the advective heat transport in the subsurface. However, the 574 flow velocity on average is quite low within the shallow active layer with limited thickness (see 575 Figure S4.1 in Supplement). This result in that the advective heat transport only makes contributions within the top shallow layers, and the relatively larger advective heat flux is lower 576 577 than the conductive heat flux over one order of magnitude (see Figure S4.2 in Supplement).



578 Therefore, for such large-scale Arctic systems where localized groundwater flow makes less

579 contributions, for most Arctic systems at this scale, it is reasonable to neglect advective heat

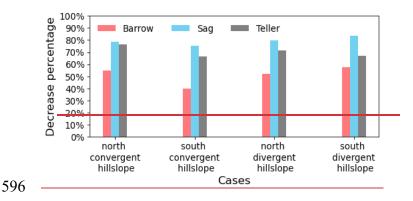
580 transport.

Figure 10 Comparison of hillslope simulations between including and neglecting advective heat transport
under extreme conditions of Teller, in (a) evaporation, (b) discharge, (c) thaw depth, (d) water saturation at 5
cm beneath surface, (e) surface temperature, (f) temperature at 1 m beneath surface.

565 Cin beneath surface, (c) surface temperature, (i) temperature at 1 in beneath surface.

586 In addition to simulated results, we also compared simulation times in percentage change between

587 hillslope models neglecting and including heat advection. ATS uses Algebraic Multigrid method 588 as preconditioner for solving, which has a relatively deficient performance in dealing with 589 hyperbolic equations. Thus, incorporating advective heat transport will aggravate computational 590 cost, particularly in case of both large spatial and temporal scale. Figure 12 shows the relative 591 percentage reduction in computational time for 10-year simulations after excluding heat advection 592 in both surface and subsurface thermal flux. It drops by 70% ~ 80% under wet conditions (e.g., 593 Sag and Teller) and 40% ~ 60% under dry conditions (e.g., Barrow). Hence, neglecting advective heat transport considerably improves the performance of large spatial-temporal permafrost 594 595 hydrology simulations.



597 Figure 12 Decreased percentage of simulation time after neglecting heat advection compared to full thermal
 598 representation for all hillslope scale simulations.

599 4.4 Comprehensive comparison

600 In the above three sections, we discussed time-series simulation comparisons. This section will 601 analyze the effect of equal ice-liquid density, neglecting cryosuction, and neglecting heat 602 advection on permafrost modeling outputs from holistic, average perspectives.

603 First, we extracted NNSEs of all variables the metrics of interest obtained from all comparing 604 models for qualitative analysis. Table 6 shows an example based on column-scale models under 605 conditions of three different sites. Red numbers highlight the obviously reduced NNSEs of one or 606 two processes among the three for each variablemetric. Overall, neglecting advective heat 607 transport has the least influence on model outputs. Equal ice-liquid density primarily affects 608 saturation and has less effect on other variables metrics. Excluding soil cryosuction makes the 609 greatest impact on almost all variables<u>metrics</u>, especially in a relatively wet environment. Among 610 these metrics variables, evaporation and surface temperature are less affected by the three physical 611 process representations, while location-based water saturation is most affected.

		Barrow			Sag		<u>Teller</u>			
<u>Metrics</u>	<u>Heat</u> advection	<u>Ice</u> <u>density</u>	<u>Cryosuction</u>	<u>Heat</u> advection	<u>Ice</u> <u>density</u>	<u>Cryosuction</u>	<u>Heat</u> advection	<u>Ice</u> density	Cryosuction	
Evaporation	<u>0.997</u>	<u>0.994</u>	<u>0.899</u>	<u>0.993</u>	<u>0.992</u>	<u>0.937</u>	<u>0.999</u>	<u>0.996</u>	<u>0.903</u>	
<u>Discharge</u>	0.924	<u>0.628</u>	0.862	<u>0.996</u>	<u>0.938</u>	<u>0.631</u>	<u>0.985</u>	<u>0.987</u>	<u>0.618</u>	
Thaw depth	<u>0.997</u>	<u>0.996</u>	<u>0.852</u>	<u>0.991</u>	<u>0.979</u>	0.904	<u>0.997</u>	<u>0.989</u>	<u>0.952</u>	
<u>5cm-depth s_w</u>	<u>0.996</u>	<u>0.934</u>	<u>0.785</u>	<u>0.992</u>	<u>0.726</u>	<u>0.926</u>	<u>0.998</u>	<u>0.562</u>	<u>0.869</u>	
<u>40cm-depth sw</u>	<u>0.993</u>	0.022	<u>0.213</u>	<u>0.995</u>	<u>0.062</u>	<u>0.311</u>	<u>0.999</u>	0.281	<u>0.850</u>	
Surface T	<u>1.000</u>	1.000	<u>0.987</u>	<u>0.999</u>	<u>0.999</u>	0.864	<u>1.000</u>	1.000	<u>0.955</u>	
<u>1m-depth T</u>	1.000	<u>1.000</u>	0.921	<u>1.000</u>	<u>1.000</u>	<u>0.613</u>	<u>1.000</u>	<u>0.999</u>	0.737	

612 Table 6 A summary of NNSEs of variables-metrics of interest obtained through column model comparison

613

		Barrow			Sag		Teller			
Variables	Heat advection	Ice density	Cryosuction	Heat advection	Ice density	Cryosuction	Heat advection	Ice density	Cryosuction	
Evaporation	0.9971	0.9942	0.8991	0.9926	0.9917	0.9365	0.9989	0.9958	0.9033	
Discharge	0.9235	0.6282	0.8615	0.9962	0.9377	0.6305	0.9854	0.9874	0.6175	
Thaw depth	0.9970	0.9961	0.8517	0.9910	0.9791	0.9036	0.9969	0.9887	0.9524	
5cm-depth sw	0.9959	0.9335	0.7851	0.9916	0.7260	0.9260	0.9979	0.5618	0.8690	
40cm-depth sw	0.9932	0.0221	0.2130	0.9951	0.0622	0.3111	0.9990	0.2807	0.8498	
Surface T	0.9999	0.9999	0.9871	0.9993	0.9990	0.8642	0.9999	0.9996	0.9554	
1m depth T	0.9999	0.9999	0.9207	0.9997	0.9996	0.6127	0.9997	0.9991	0.7366	

 $614 * s_w$ and T in Table 6 are water saturation and temperature, respectively.

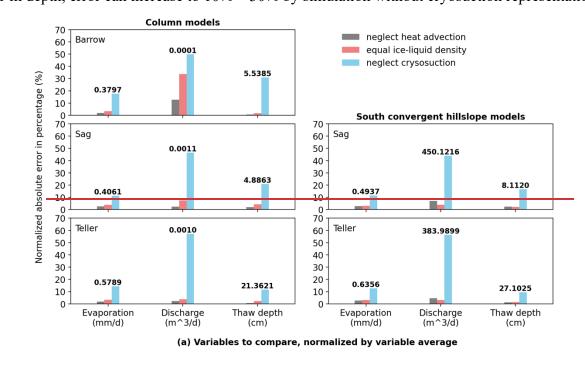
Furthermore, to quantitively compare across the physical processess quantitively, we calculated 615 the mean absolute error (MAE) for each variable-metric of interest over the simulation period of 616 2011-2020. For evaporation, discharge, and thaw depth, the MAEs are normalized by the 617 618 corresponding variable metric average (numbers in Figure 11 (a)); for water saturation and 619 temperature, the MAEs are normalized by their average annual fluctuation range (numbers in 620 Figure 11 (b)). All normalized MAEs are presented in percentage, displayed in Figure 11 according 621 to column- and hillslope-scale (e.g., south-facing convergent hillslope) models under three 622 different climate conditions. Hillslope-scale model output under conditions of Barrow is not shown 623 in that flat land occupies a majority of the area. A larger normalized MAE percentage indicates greater impact on the variable metric resulted from a physical process. 624

From the perspective of 10-year average, in general, each physical process of Arctic systems discussed in this paper presents a similar impact on variables-metrics between column and hillslope scales. Under climate and soil conditions of three different sites, neglecting cryosuction in permafrost modeling leads to the greatest influence on hydrological prediction amongst the three

629 physical assumptions. As seen in Figure 11 (a), it will result in $10\% \sim 20\%$ deviation in evaporation,

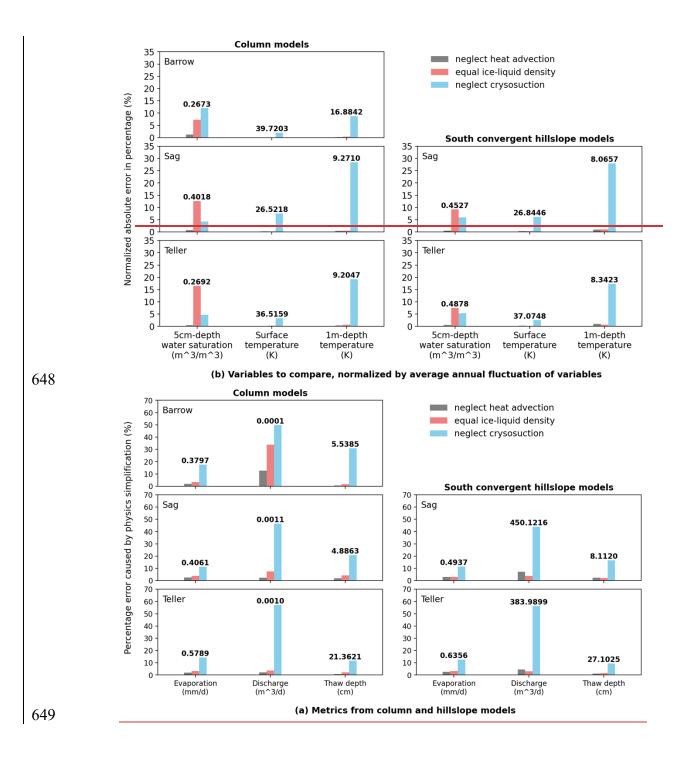
630 $50\% \sim 60\%$ in discharge, and $10\% \sim 30\%$ in that depth. Evaporation is the least affected among 631 the three variables metrics. Discharge is more affected in regions with abundant rainfall (Teller), 632 while in regions with less precipitation, evaporation and thaw depth are relatively affected 633 (Barrow). By comparison, assuming equal ice-liquid density and neglecting advective heat transport may only cause 10% and 5% or even much lower error, respectively, in reference to the 634 635 annual average of a metricvariable. Specially in Barrow, models utilizing the same ice and liquid 636 densities and ignoring advective heat transport seem to make an obvious impact on discharge, whereas this also results from its extremely low discharge (Figure 6 (b)). 637

638 Figure 11 (b) illustrates the normalized MAEs of water saturation at 5 cm beneath surface, as well 639 as temperature at surface and 1 m depth. The assumption of equal ice-liquid density primarily 640 affects the estimation of the water saturation profiles, which. It can lead to about $5\% \sim 15\%$ error 641 relative to the annual change range, and the error percentage tends to slightly decrease when 642 applying hillslope-scale models due to the inclusion of lateral flow. Apart from this, neglecting 643 soil cryosuction still makes the largest impact. Surface temperature is the least affected variable 644 metric among all these model outputs even if cryosuction is not included in modeling. However, 645 at 1 m depth, error can increase to $10\% \sim 30\%$ by simulation without cryosuction representation.



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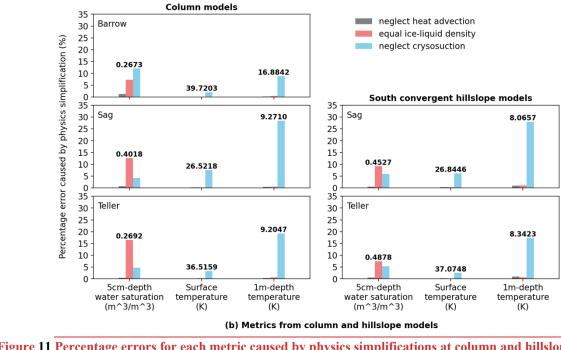


Figure 11 Percentage errors for each metric caused by physics simplifications at column and hillslope scales.
 The percentage error refers to the averaged error of a metric over the period of 2011-2020 normalized by a
 certain reference value obtained from full-physics model. Metrics include (a) evaporation, discharge, and
 thaw depth; (b) water saturation, and temperatures. Numbers in figures are the corresponding reference
 values for each metric: (a) 10-year average obtained from full-physics model; (b) 10-year averaged annual
 fluctuation range obtained from full-physics model.

657 **5 Conclusion**

650

658 The premise of this study is, by starting from general mass and energy transport equations and 659 simplifying the process representations, we can use a process-rich model to understand the relative 660 importance of given process simplifications in describing permafrost hydrology. This process 661 sensitivity analysis, performed at the scale of field sites as opposed to previous studies at smaller 662 scales such as lab experiments, provides improved understanding in the processes governing 663 permafrost hydrology at this scale. As the simplifications considered here largely span the 664 equations considered in a class of process-rich models, this process sensitivity analysis is relevant 665 to model developers across a range of codes. 666 Simplification of Arctic process representation is an essential consideration when developing 667 process-rich models for thermal permafrost hydrology. There are following three subsurface 668 process simplificationses that are commonly described applied in a simplified approach for many 669 Arctic tundra models: (i) ice is prescribed the same density as liquid water; (ii) the effect of soil 670 cryosuction is neglected; (iii) advective heat transport is neglected. Here we investigated the 671 influence of these simplified representations on modeling field-scale permafrost hydrology in set

672 of simplified geometries commonly used in the permafrost hydrology literature with the Advanced

673 Terrestrial Simulator (ATS v1.2). We note that these conclusions are specific to conditions similar

674 to these geometries, and should not be applied in cases where focusing flow mechanisms may675 dominate.

676 To do this, we conducted an ensemble of simulations using the Advanced Terrestrial Simulator 677 (ATS v1.2) to evaluate the impact of the above three process simplifications on field-scale predictions. The ensemble of simulations consisted of 62 numerical experiments considering 678 679 various conditions, including different climate conditions and soil properties at three sites of 680 Alaska, and different model scale conceptualizations. For evaluation, we compared integrated 681 variables metrics (evaporation, discharge), averaged thaw depth, and pointwise variables metrics 682 (temperature, total water saturation), which are of general interest, among different models to 683 access the deviation of applying a simplified modeling assumption. The main conclusions, under 684 the assumed conditions inof this study, are summarized as follows:

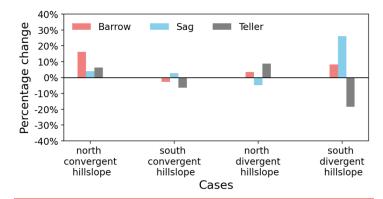
685 1) Excluding soil cryosuction in permafrost models can cause significant bias on estimation 686 of in-most hydrological variables metrics at field-scale permafrost simulations. Especially, 687 according to In particular, under the assumed conditionsthis study, the average deviation 688 in evaporation, discharge, and thaw depth may reach $10\% \sim 20\%$, $50\% \sim 60\%$, and $10\% \sim 10\%$ 689 30%, respectively, relative to the corresponding annual average values. The prediction 690 error for discharge may grow if rainfall rates increase. In the case of pointwise 691 variables metrics, the error in temperature increases from a small amount at the surface up to $10\% \sim 30\%$ at 1 m beneath surface. The prediction of subsurface temperature and water 692 693 saturation is especially affected when considering hillslope scale models. Therefore, soil 694 cryosuction should be included when modeling permafrost change.

Assuming equal ice-liquid density will not result in especially large deviations when
predicting most of the hydrological variablesmetrics, particularly at hillslope scales given
all cases in this study. It primarily affects the prediction of the soil water saturation profile
and can cause 5% ~ 15% error relative to the annual saturation fluctuation range. This
difference may have consequences for the carbon cycle with regards to the production of
methane versus carbon dioxide. Assigning liquid water density for ice may reduce
computational time to a small extent in ATS, dependent on simulating conditions and

- 702 spatial and temporal scales.
- 3) For a large-scale general-Arctic tundra system with limited localized groundwater flow
 features (e.g., taliks, thermo-erosion gullies, etc.), the prediction error in most variables
 metrics of interest after neglecting advective heat transport is less than 5%, or even much
 lower. In the case of ATS, the simulation time cost for hillslope-scale models can decrease
 by 40% to 80% under conditions in this study. Ignoring heat advection in the absence of
 local, flow-focusing mechanisms, such as thermo-erosion gullies, seems a reasonable
 decision.
- 710 Through the comparison of permafrost hydrological outputs obtained from ensemble model setups 711 targeted at the field scale, we confirm the importance and necessity of including soil cryosuction 712 effect in predicting permafrost changes, and validate the application of equal ice-liquid density and neglecting advective heat transport for an general Arctic system where localized groundwater 713 714 flow is not a dominant feature. The latter two may also ease computational cost dependent upon 715 simulation conditions. We expect that this study can contribute to the development of permafrost 716 hydrology models, as well as better selection of physical process representations for modelers, and 717 better understanding of permafrost physics for the community.

718 Appendix

- 719 The following results may provide some information about computation cost for ATS users. In
- 720 addition to the influence of process representations on permafrost hydrology metrics of general
- 721 interest, we also investigated how much the simplified processes can affect the runtime of a model
- 722 at the hillslope scale.
- 723 First, using the 10-year simulation with real ice density as references, the percentage change of
- 724 time consumed after applying equal ice-liquid density was calculated and displayed in Figure A1.
- 725 Overall, under the equal density assumption, it may take less time (positive values in figure), but
- 726 no more than 25% and on average lower than 10%. However, the computation time may also
- 727 increase (negative values in figure) under wet conditions, such as at Sag and Teller. Thus, given a
- 728 long-period modeling of large-scale permafrost system, there is no consistent conclusion on
- 729 whether equal ice-liquid density can ease computational cost. It depends on both the weather
- 730 conditions and soil properties.





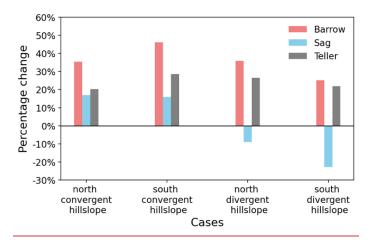
- Figure A1. The relative runtime change in percentage due to the assumption of equal ice-liquid density
 compared to that with the real ice density representation for all hillslope scale models.
- 734 Second, section 4.2 has demonstrated that neglecting cryosuction will make a great impact on

735 hydrological estimations. As a significant physical process of permafrost, cryosuction should be

736 implemented in numerical models even if additional computation effort is potentially required.

737 However, based on the hillslope models we conducted, including cryosuction does not necessarily

- 738 raise computational cost, which also depends on specific soil properties and conditions. The cases
- 739 <u>that consume more time after considering cryosuction effect just increase the time by $10\% \sim 30\%$ </u>,
- 740 and less than 20% on average (see Figure A2).



741



⁷⁴⁴ Third, in terms of heat advection, ATS uses the Algebraic Multigrid method as preconditioner for

- 745 solving, which has a relatively deficient performance in dealing with hyperbolic equations. Thus,
- 746 incorporating advective heat transport will aggravate computational cost, particularly in case of
- 747 both large spatial and temporal scales. Figure A3 shows the relative percentage reduction in
- 748 computational time for 10-year simulations after excluding heat advection in both surface and

- 749 subsurface thermal flux. It drops by 70% ~ 80% under wet conditions (e.g., Sag and Teller) and
- 750 40% ~ 60% under dry conditions (e.g., Barrow). Hence, neglecting advective heat transport
- 751 considerably improves the performance of large spatial-temporal permafrost hydrology
- 752 simulations.

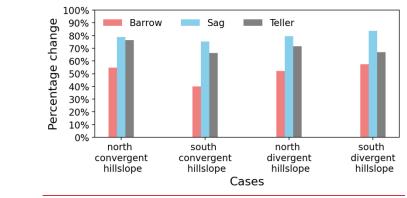


Figure A3. The relative runtime change in percentage due to the neglect of advective heat transport for all
 hillslope scale models.

756 Code availability

753

757 Advanced Terrestrial Simulator (ATS) is an open-source code for solving ecosystem-based,

- 758 integrated, distributed hydrology, and available at <u>https://github.com/amanzi/ats</u>. Simulations were
- 759 conducted using version 1.2 (Coon et al., 2021).

760 Data availability

- 761 Data sources of wind speed are cited in the text. The raw forcing data acquired from Daymet, the
- 762 processed forcing data used for simulation, and simulation output data are available through
- 763 <u>https://github.com/gaobhub/data_for_paper_model_comparison</u>.

764 Author contributions

- 765 Bo Gao did some revision of the code to add options for process representations, designed
- 766 numerical experiments and setup models, did data analysis and interpretation, drafted and revised
- 767 the article. Ethan T. Coon implemented the code in which the study was done, conceptualized the
- 768 study, helped debug the runs, and helped draft and revise the article.

769 Competing interests

770 The authors declare that they have no conflict of interest.

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