1 Sensitivity of airborne geophysical data to sublacustrine

2 and near-surface permafrost thaw

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Abstract

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A coupled hydrogeophysical forward and inverse modeling approach is developed to illustrate the ability of frequency-domain airborne electromagnetic (AEM) data to characterize subsurface physical properties associated with sublacustrine permafrost thaw during lake talik formation. Numerical modeling scenarios are evaluated that consider non-isothermal hydrologic responses to variable forcing from different lake depths and for different hydrologic gradients. A novel physical property relationship connects the dynamic distribution of electrical resistivity to ice-saturation and temperature outputs from the SUTRA groundwater simulator with freeze/thaw physics. The influence of lithology on electrical resistivity is controlled by a surface conduction term in the physical property relationship. Resistivity models, which reflect changes in subsurface conditions, are used as inputs to simulate AEM data in order to explore the sensitivity of geophysical observations to permafrost thaw. Simulations of sublacustrine talik formation over a 1,000-year period are modeled after conditions found in the Yukon Flats, Alaska. Synthetic AEM data are analyzed with a Bayesian Markov chain Monte Carlo algorithm that quantifies geophysical parameter uncertainty and resolution. Major lithological and permafrost features are well resolved by AEM data in the examples considered. The subtle geometry of partial ice-saturation beneath lakes during talik formation cannot be resolved using AEM data, but the gross characteristics of sub-lake resistivity models reflect bulk changes in ice content and can identify the presence of a talik. A final synthetic example compares AEM and ground-based electromagnetic responses for their ability to resolve shallow permafrost and thaw features in the upper 1-2 m below ground outside the lake margin.

1 Introduction

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45 Permafrost thaw can have important consequences for the distribution of surface water 46 (Roach et al., 2011; Rover et al., 2012), stream discharge and chemistry (O'Donnell et 47 al., 2012; Petrone et al., 2007; Striegl et al., 2005; Walvoord and Striegl, 2007), and 48 exchange between groundwater and surface water systems (Bense et al., 2009; Callegary 49 et al., 2013; Walvoord et al., 2012). Likewise, hydrologic changes that alter the thermal 50 forcing supplied by surface water or groundwater systems can modify the distribution of 51 permafrost, illustrating the strong feedbacks between permafrost and hydrology. In 52 addition to hydrologic processes, permafrost is affected by climate warming in Arctic and 53 sub-Arctic regions (Hinzman et al., 2005; Jorgenson et al., 2001), as well as disturbance 54 by fire (Yoshikawa et al., 2002). Climate feedbacks associated with permafrost thaw 55 include changes in the amount of organic carbon stored in soils that is vulnerable to 56 decomposition (Koven et al., 2011; O'Donnell et al., 2011) and subsequent methane and 57 carbon dioxide released from soils by the degradation of organic material previously 58 sequestered in frozen ground (Anthony et al., 2012). Permafrost thaw also has significant 59 implications for land management and infrastructure, including the potential to damage 60 buildings, roadways, or pipelines due to ground settling, and thermal erosion that can 61 alter coastlines and landscape stability (Larsen et al., 2008; Nelson et al., 2002). 62 Several investigations have shown the significance of climate and advective heat 63 transport in controlling the distribution of permafrost in hydrologic systems (Bense et al., 64 2009; Rowland et al., 2011; Wellman et al., 2013). These results yield important insight 65 into the mechanistic behavior of coupled thermal-hydrologic systems, and are a means 66 for predicting the impact on permafrost from a wide range of climate and hydrologic 67 conditions. However, few techniques are capable of assessing the distribution of 68 permafrost, and most approaches only capture a single snapshot in time. 69 Satellite remote-sensing techniques have proven useful in detecting the distribution and 70 changes in shallow permafrost, vegetation, and active layer thickness over large areas 71 (Liu et al., 2012; Panda et al., 2010; Pastick et al., 2014), but are only sensitive to very 72 near-surface properties. Borehole cores and downhole temperature or geophysical logs 73 provide direct information about permafrost and geologic structures, but tend to be

74 sparsely located and are not always feasible in remote areas. Geophysical methods are 75 necessary for investigating subsurface physical properties over large and/or remote areas. 76 Recent examples of geophysical surveys aimed at characterizing permafrost in Alaska 77 include: an airborne electromagnetic (AEM) survey used to delineate geologic and 78 permafrost distributions in an area of discontinuous permafrost (Minsley et al., 2012), 79 ground-based electrical measurements used to assess shallow permafrost aggradation 80 near recently receded lakes (Briggs et al., 2014), electrical and electromagnetic surveys 81 used to characterize shallow active layer thickness and subsurface salinity (Hubbard et al., 2013), and surface nuclear magnetic resonance (sNMR) soundings used to infer the 82 83 thickness of unfrozen sediments beneath lakes (Parsekian et al., 2013). A challenge with 84 geophysical methods, however, is that geophysical properties (e.g. electrical resistivity) 85 are only indirectly sensitive to physical properties of interest (e.g. lithology, water 86 content, thermal state). In addition, various physical properties can produce similar 87 electrical resistivity values. Therefore, it is critically important to understand the 88 relationship between geophysical properties and the ultimate physical properties and 89 processes of interest (Minsley et al., 2011; Rinaldi et al., 2011). 90 The non-isothermal hydrologic simulations of Wellman et al. (2013) predict the evolution 91 of lake taliks (unfrozen sub-lacustrine areas in permafrost regions) in a two-dimensional 92 axis-symmetric model under different environmental scenarios (e.g. lake size, climate, 93 groundwater flow regime). Here, we investigate the ability of geophysical measurements 94 to recover information about the underlying spatial distribution of permafrost and 95 hydrologic properties. This is accomplished in three steps: (1) development of a physical 96 property relation that connects permafrost and hydrologic properties to geophysical 97 properties; (2) generation of synthetic geophysical data that would be expected for 98 various permafrost hydrologic conditions that occur during simulated lake talik 99 formation; and (3) inversion of the synthetic geophysical data using realistic levels of 100 noise to investigate the ability to resolve specific physical features of interest. Our focus 101 is on electromagnetic geophysical methods as these types of data have previously been 102 acquired near Twelvemile Lake in the Yukon Flats, Alaska (Ball et al., 2011; Minsley et 103 al., 2012); a lake that is also the basis for the lake simulations discussed by Wellman et 104 al. (2013).

2 Methods

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described below.

106 2.1 **Coupled Thermal-hydrologic Simulations** 107 Wellman et al. (2013) describe numerical simulations of lake-talik formation in 108 watersheds modeled after those found in the lake-rich Yukon Flats of interior Alaska. 109 Modeling experiments used the SUTRA groundwater modeling code (Voss and Provost, 110 2002) enhanced with capabilities to simulate freeze-thaw processes (McKenzie and Voss, 111 2013). The phase change between ice and liquid water occurs over a specified 112 temperature range, and accounts for latent heat of fusion as well as changes in thermal 113 conductivity and heat capacity for ice-water mixtures. Ice content also changes the 114 effective permeability, thereby altering subsurface flowpaths and enforcing a strong 115 coupling between hydraulic and thermal processes. The modeling domain, which is 116 adapted for this study, is axis-symmetric with a central lake and upwards-sloping ground 117 surface that rises from an elevation of 500 m at r = 0 m to 520 m at the outer extent of the 118 model, r = 1800 m (Figure 1). The model uses a layered-geology consistent with the 119 Yukon Flats (Minsley et al., 2012; Williams, 1962), with defined hydrologic and 120 geophysical parameters for each layer summarized in Table 1. Initial permafrost 121 conditions prior to lake formation were established by running the model to steady state 122 under hydrostatic conditions with a constant temperature of -2.25 °C applied to the land 123 surface, which produces a laterally continuous permafrost layer extending to a depth of 124 about 90 m. 125 Subsequent hydrologic simulations assume fully saturated conditions, and are performed 126 over a 1,000-year period under 36 different scenarios of climate (warmer than, colder 127 than, and similar-to present conditions); hydrologic gradient (hydrostatic, gaining, and 128 losing lake conditions); and lake depth/extent (3-, 6-, 9-, and 12-m-deep lakes that 129 intersect the ground surface at increasing distance, as shown in Figure 1). Complete 130 details and results of the hydrologic simulations can be found in Wellman et al. (2013). 131 At each simulation time step, the SUTRA model outputs temperature, pressure, and ice 132 saturation. Conversion of these hydrologic variables to electrical resistivity- the 133 geophysical property needed to simulate electromagnetic data considered here- is

2.2 A physical property relationship

- 136 Electrical resistivity is the primary geophysical property of interest for the 137 electromagnetic geophysical methods used in this study. It is well-established that 138 resistivity is sensitive to basic physical properties such as unfrozen water content, soil or 139 rock texture, and salinity (Palacky, 1987). Here, we build on earlier efforts to simulate 140 the electrical properties of ice-saturated media (Hauck et al., 2011) by using a modified 141 form of Archie's Law (Archie, 1942) that also incorporates surface conduction effects 142 (Revil, 2012) to predict the dynamic electrical resistivity structure for the evolving state
- 143 of temperature and ice saturation (S_i) in the talik simulations. Bulk electrical
- 144 conductivity is described by Revil (2012) as

$$\sigma = \frac{S_w^n}{F} \left[\sigma_f + m \left(S_w^{-n} F - 1 \right) \sigma_s \right], \tag{1}$$

- where σ is the bulk electrical conductivity [S/m]; S_w is the fractional water saturation [-] 146
- 147 in the pore space, where $S_w = 1 - S_i$; σ_f is the conductivity of the saturating pore fluid
- [S/m]; m is the Archie cementation exponent [-]; n is the Archie saturation exponent [-]; 148
- F is the formation factor [-], where $F = \phi^{-m}$ and ϕ is the matrix porosity [-]; and σ_s is the 149
- 150 conductivity [S/m] associated with grain surfaces. The Archie exponents m and n are
- known to vary as a function of pore geometry; here, we use m = n = 1.5, which is 151
- 152 appropriate for unconsolidated sediments (Sen et al., 1981). Simulation results are
- 153 presented as electrical resistivity [ohm-m], which is the inverse of the conductivity, i.e. p
- 154 $= 1/\sigma$.

- 155 The first term in Eq. (1) describes electrical conduction within the pore fluid, where fluid
- 156 conductivity is defined as

$$\sigma_f = F_c \sum_i \beta_i |z_i| C_i . \tag{2}$$

- The summation in Eq. (2) is over all dissolved ionic species (Na⁺ and Cl⁻ are assumed to 158
- 159 be the primary constituents in this study), where F_c is Faraday's constant [C/mol] and C_i ,
- β_i , and z_i are the concentration [mol/L], ionic mobility [m²/Vs], and valence of the i^{th} 160
- 161 species, respectively.

Surface conduction effects, described by the second term in Eq. (1), are related to the chemistry at the pore-water interface, and can be important in fresh water (low conductivity) systems at low porosity (high ice saturation). Additionally, the surface conduction term provides a means for describing the conductivity behavior for different lithologies, as will be described below. The surface conductivity is given by

$$\sigma_{s} = \frac{2}{3} \left(\frac{\phi}{1 - \phi} \right) \beta_{s} Q_{v} , \qquad (3)$$

- where β_s is the cation mobility [m²/Vs] for counterions in the electrical double layer at the
- grain-water interface (Revil et al., 1998) and Q_v is the excess electrical charge density
- 170 $[C/m^3]$ in the pore volume,

$$Q_{v} = S_{w}^{-1} \rho_{g} \left(\frac{1 - \phi}{\phi} \right) \chi , \qquad (4)$$

- where ρ_g is the mass density of the grains [kg/m³] and χ is the cation exchange capacity
- 173 [C/kg]. Changes in χ, representative of bulk differences in clay mineral content, are used
- to differentiate the electrical signatures of the lithologic units in this study (Table 1).
- The temperature, T[C], dependence of ionic mobility affects both the fluid conductivity
- 176 (Eq. (2)) and surface conductivity (Eq. (3)), where mobility is approximated as a linear
- 177 function of temperature (Keller and Frischknecht, 1966; Sen and Goode, 1992) as

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$$\beta(T) = \beta_{T=25C} [1 + 0.019(T - 25)]. \tag{5}$$

- 179 Finally, we consider the effect of increasing ice saturation on salinity. Because salts are
- generally excluded as freezing occurs, salinity of the remaining unfrozen pore water is
- expected to increase with increasing ice content (Marion, 1995), leading to a
- 182 corresponding increase in fluid conductivity according to Eq. (2). To describe this
- dependence of salinity on ice saturation, $C(S_i)$, we use the expression

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$$C(S_i) = C_{S_i=0} S_w^{-\alpha}$$
 (6)

- where $\alpha \sim 0.8$ accounts for loss of solute from the pore space due to diffusion or other
- transport processes, and $S_i = 1 S_w$.

187 Information about the different lithologic units described by Wellman et al. (2013) that 188 are also summarized in Table 1 are used to define static model properties such as 189 porosity, grain mass density, cation exchange capacity, and Archie's exponents. 190 Dynamic outputs from the SUTRA simulations, including temperature and ice saturation, 191 are combined with the static variables in Eqs. (1) - (6) to predict the evolving electrical 192 resistivity structure. 193 2.3 **Geophysical Forward Simulations** 194 Synthetic airborne electromagnetic (AEM) data are simulated for each snapshot of 195 predicted bulk resistivity values using nominal system parameters based on the Fugro 196 RESOLVE¹ frequency-domain AEM system that was used in the Yukon Flats survey 197 (Minsley et al., 2012). The RESOLVE system consists of five horizontal coplanar (HCP) 198 transmitter-receiver coil pairs separated by approximately 7.9 m that operate at 199 frequencies 0.378 kHz, 1.843 kHz, 8.180 kHz, 40.650 kHz, and 128.510 kHz; and one 200 vertical coaxial (VCX) coil pair with 9-m separation that operates at 3.260 kHz. 201 Oscillating currents and associated magnetic fields created by the transmitter coils induce 202 electrical currents in the subsurface that, in turn, generate secondary magnetic fields that 203 are recorded by the receiver coils (Siemon, 2006; Ward and Hohmann, 1988). Data are 204 reported as in-phase and quadrature components of the secondary field in parts-per-205 million (ppm) of the primary field, and responses as a function of frequency can be 206 converted through mathematical inversion to estimates of electrical resistivity as a 207 function of depth (e.g., Farguharson et al., 2003). Data are simulated at the nominal 208 survey elevation of 30 m above ground surface using the one-dimensional modeling 209 algorithm described in Minsley (2011), which follows the standard electromagnetic 210 theory presented by Ward and Hohmann (1988). 211 The vertical profile of resistivity as a function of depth is extracted at each survey 212 location and is used to simulate forward geophysical responses. There are 181 sounding 213 locations for each axis-symmetric model, starting at the center of the lake (r = 0 m) to the

 $^{\rm 1}$ Any use of trade, product, or firm names is for descriptive purposes only and does not imply endorsement by the U.S. Government

edge of the model domain (r = 1,800 m) in 10-m increments. Each vertical resistivity

215 profile extends to 200 m depth, which is well beyond the depth to which we expect to 216 recover parameters in the geophysical inversion step. A center-weighted 5-point filter 217 with weights equal to [0.0625, 0.25, 0.375, 0.25, 0.0625] is used to average neighboring 218 bulk resistivity values at each depth before modeling in order to partly account for the 219 lateral sensitivity of AEM systems (Beamish, 2003). Forward simulations are repeated 220 for each of the 50 simulation times between 0 and 1,000 years output from SUTRA, 221 resulting in 9,050 data locations per modeling scenario. 222 Synthetic ground-based electromagnetic data presented in Section 3.3 are simulated using 223 nominal system parameters based on the GEM-2 instrument (Huang and Won, 2003). 224 The GEM-2 has a single HCP transmitter-receiver pair separated by 1.66 m, and data are 225 simulated at six frequencies: 1.5 kHz, 3.5 kHz, 8.1 kHz, 19 kHz, 43 kHz, and 100 kHz. 226 A system elevation of 1 m above ground is assumed, which is typical for this hand-227 carried instrument. 228 2.4 **Parameter Estimation and Uncertainty Quantification** 229 The inverse problem involves estimating subsurface resistivity values given the simulated 230 forward responses and realistic assumptions about data errors. Geophysical inversion is 231 inherently uncertain; there are many plausible resistivity models that are consistent with 232 the measured data. In addition, the ability to resolve true resistivity values is limited both 233 by the physics of the AEM method and the level of noise in the data. Here, we use a 234 Bayesian Markov chain Monte Carlo (McMC) algorithm developed for frequency-235 domain EM data (Minsley, 2011) to explore the ability of simulated AEM data to recover 236 the true distribution of subsurface resistivity values at 20-year intervals within the 1,000-237 year lake talik simulations. This McMC approach is an alternative to traditional 238 inversion methods that find a single 'optimal' model that minimizes a combined measure 239 of data fit and model regularization (Aster et al., 2005). Although computationally more 240 demanding, McMC methods allow for comprehensive model appraisal and uncertainty 241 quantification. AEM-derived resistivity estimates for the simulations considered here 242 will help guide interpretations of future field datasets, identifying the characteristics of 243 relatively young versus established thaw under different hydrologic conditions.

244	The McMC algorithm provides comprehensive model assessment and uncertainty		
245	analysis, and is useful in diagnosing the ability to resolve various features of interest. At		
246	every data location along the survey profile, an ensemble of 100,000 resistivity models is		
247	generated according to the Metropolis-Hastings algorithm (Hastings, 1970; Metropolis et		
248	al., 1953). According to Bayes' theorem, each model is assigned a posterior probability		
249	that is a measure of (1) its prior probability which, in this case, is used to penalize models		
250	with unrealistically large contrasts in resistivity over thin layers; and (2) its data		
251	likelihood, which is a measure of how well the predicted data for a given resistivity		
252	model match the observed data within data errors. A unique aspect of this algorithm is		
253	that it does not presuppose the number of layers needed to fit the observed data, which		
254	helps avoid biases due to assumptions about model parameterization. Instead, trans-		
255	dimensional sampling rules (Green, 1995; Sambridge et al., 2013) are used to allow the		
256	number of unknown layers to be one of the unknowns. That is, the unknown parameters		
257	for each model include the number of layers, layer interface depths, and resistivity values		
258	for each layer.		
259	Numerous measures and statistics are generated from the ensemble of plausible resistivity		
260	models, such as: the single most-probable model, the probability distribution of resistivity		
261	values at any depth, the probability distribution of where layer interfaces occur as a		
262	function of depth, and the probability distribution of the number of layers (model		
263	complexity) needed to fit the measured data. A detailed description of the McMC		
264	algorithm can be found in Minsley (2011). Finally, probability distributions of resistivity		
265	are combined with assumptions about the distribution of resistivity values for any		
266	lithology and/or ice content in order to make a probabilistic assessment of lithology or ice		
267	content, as illustrated below.		
268	3 Results		
269	3.1 Electrical resistivity model development		

Electrical resistivity model development 3.1

- 270 Information about the different lithologic units described by Wellman et al. (2013) that
- are also summarized in Table 1 are used to define static model properties such as 271
- 272 porosity, grain mass density, cation exchange capacity, and Archie's exponents.
- Dynamic outputs from the SUTRA simulations, including temperature and ice saturation, 273

274 are combined with the static variables in Eqs. (1) - (6) to predict the evolving electrical 275 resistivity structure. The behavior of bulk resistivity as a function of ice saturation is 276 shown in Figure 2. Separate curves are shown for a range of χ (cation exchange capacity) 277 values, which are the primary control in defining offset resistivity curves for different 278 lithologies, where increasing γ is generally associated with more fine-grained material 279 such as silt or clay. 280 For each of the 1,000-year simulations, the static variables summarized in Table 1 are 281 combined with the spatially and temporally variable state variables T and S_i output by 282 SUTRA to predict the distribution of bulk resistivity at each time step using Eqs. (1) - (6). 283 An example of SUTRA output variables for the 6 m-deep gaining lake scenario at 240 284 years (the approximate sub-lake talik breakthrough time for that scenario) is shown in 285 Figure 3A-B, and the predicted resistivity for this simulation step is shown in Figure 3C. 286 The influence of different lithologic units is clearly manifested in the predicted resistivity 287 values, whereas lithology is not overly evident in the SUTRA state variables. For a 288 single unit, there is a clear difference in resistivity for frozen versus unfrozen conditions. 289 Across different units, there is a contrast in resistivity when both units are frozen or 290 unfrozen. Resistivity can therefore be a valuable indicator of both geologic and ice 291 content variability. However, there is also ambiguity in resistivity values as both 292 unfrozen Unit 2 and frozen Unit 3 appear to have intermediate resistivity values of 293 approximately 100-300 ohm-m (Figure 3C) and cannot be characterized by their 294 resistivity values alone. This ambiguity in resistivity can only be overcome by additional 295 information such as borehole data or prior knowledge of geologic structure. Synthetic 296 bulk resistivity values according to Eq. (1) are shown in Figure 4 for the four different 297 lake depths (3, 6, 9, and 12 m) at three different simulation times (100, 240, and 1,000 298 years) output from the hydrostatic/current climate condition simulations. 299 Lithology and ice saturation are the primary factors that control simulated resistivity 300 values (Figure 2), though ice saturation is a function of temperature. The empirical 301 relation between temperature and bulk resistivity is shown in Figure 3D by cross-plotting 302 values from Figure 3B-C. Within each lithology resistivity is relatively constant above 303 zero degrees, with a rapid increase in resistivity for temperatures below zero degrees. 304 This result is very similar to the temperature-resistivity relationships illustrated by

305 Hoekstra (1975, Fig. 1), lending confidence to our physical property definitions described 306 earlier. Above zero degrees, the slight decrease in resistivity is due to the temperature-307 dependence of fluid resistivity. The rapid increase in resistivity below zero degrees is 308 primarily caused by reductions in effective porosity due to increasing ice saturation, 309 though changes in surface conductivity and salinity at increasing ice saturation are also 310 contributing factors. Below -1C, the change in resistivity values as a function of 311 temperature rapidly decreases. This is an artifact caused by the imposed temperature-ice 312 saturation relationship defined in SUTRA that, for these examples, enforces 99% ice 313 saturation at -1C. It is more likely that ice saturation continues to increase asymptotically 314 over a larger range of temperatures below zero degrees, with corresponding increases in 315 electrical resistivity. However, because AEM methods are limited in their ability to 316 discern differences among very high resistivity values, as discussed later, this artifact 317 does not significantly impact the results presented here. 318 3.2 Parameter Estimation and Uncertainty Quantification 319 AEM data (not shown) are simulated for each of the electrical resistivity models (e.g. 320 Figure 4) using the methods described in Section 2.3. The simulated data are then used to 321 recover estimates of the original resistivity values according to the approach outlined in 322 Section 2.4, assuming 4% data error with an absolute error floor of 5 ppm. Resistivity 323 parameter estimation results for the 6 m-deep hydrostatic lake scenario (Figure 4, D-F) 324 are shown in Figure 5. At each location along the profile, the average resistivity model as 325 a function of depth is calculated from the McMC ensemble of 100,000 plausible models. 326 The overall pattern of different lithologic units and frozen/unfrozen regions is accurately 327 depicted in Figure 5, with two exceptions that will be discussed in greater detail: (1) the 328 specific distribution of partial ice saturation beneath the lake before thaw has equilibrated 329 (Figure 5A-B); and (2) the shallow sand layer (Unit 1) that is generally too thin to be 330 resolved using AEM data. 331 A point-by-point comparison of true (Figure 4F) versus predicted (Figure 5C) resistivity 332 values for the hydrostatic 6 m-deep lake scenario at the simulation time 1,000 years is 333 shown in Figure 6A. The cross-plot of true versus estimated resistivity values generally 334 fall along the 1:1 line, providing a more quantitative indication of the ability to estimate

335 the subsurface resistivity structure. Estimates of the true resistivity values for each 336 lithology and freeze/thaw state (Figure 6B) tend to be indistinct; appearing as a vertical 337 range of possible values in Figure 6A due to the inherent resolution limitations of inverse 338 methods and parameter tradeoffs (Day-Lewis, F. D. et al., 2005; Oldenborger and Routh, 339 2009). Although the greatest point density for both frozen and unfrozen silts (Unit 3) 340 falls along the 1:1 line, resistivity values for these components of the model are also often 341 overestimated; this is likely due to uncertainties in the location of the interface between 342 the silt and gravel units. This is in contrast with the systematic underestimation of frozen 343 gravel resistivity values due to the inability to discriminate very high resistivity values 344 using EM methods (Ward and Hohmann, 1988). Frozen sands (true log resistivity ~2.8 345 in Figure 6B) are also systematically overestimated in Figure 6A; in this case, due to the 346 inability to resolve this relatively thin resistive layer. 347 While useful, single 'best' estimates of resistivity values at any location (Figure 6) are 348 not fully representative of the information contained in the AEM data and associated 349 model uncertainty. From the McMC analysis of 100,000 models at each data location, 350 estimates of the posterior probability density function (pdf) of resistivity are generated for 351 each point in the model. Probability distributions are extracted from a depth of 15 m. 352 within the gravel layer (Unit 2), at one location where unfrozen conditions exist (r = 0)353 m), and a second location outside the lake extent (r = 750 m) where the ground remains 354 frozen (Figure 7A). Results from a depth of 50 m, within the silt layer (Unit 3), are 355 shown in Figure 7B. With the exception of the frozen gravels, whose resistivity tends to 356 be underestimated, the peak of each pdf is a good estimate of the true resistivity value at 357 that location. 358 Resistivity values are translated to estimates of ice saturation, which is displayed on the 359 upper axis of each panel in Figure 7, using the appropriate lithology curve from Figure 2. 360 Using the ice saturation-transformed pdfs, quantitative inferences can be made about the 361 probability of the presence or absence of permafrost. For example, the probability of ice 362 content being less than 50% is estimated by calculating the fractional area under each 363 distribution for ice-content values less than 0.5. Probability estimates of ice content less 364 than 50% and greater than 95% for the four distributions shown in Figure 7 are 365 summarized in Table 2. High probabilities of ice content exceeding 95% are associated

366 with the r = 750 m location outside the lake extent, whereas high probability of ice 367 content below the 50% threshold are observed at r = 0 beneath the center of the lake. The 368 pdfs for each lithology shown in Figure 7 are end-member examples of frozen and 369 unfrozen conditions. Within a given lithology, a smooth transition from the frozen-state 370 pdf to the unfrozen-state pdf is observed as thaw occurs, with corresponding transitions in 371 the calculated ice threshold probabilities. 372 Further illustration of the spatial and temporal changes in resistivity pdfs are shown in 373 Figure 8. The resistivity pdf is displayed as a function of distance from the lake center at 374 the same depths (15 m and 50 m) shown in Figure 7, corresponding to gravel (Figure 375 **8A**,C, and E) and silt (Figure **8B**, D, and F) locations. High probabilities, i.e. the peaks in 376 Figure 7, correspond to dark-shaded areas in Figure 8. Images are shown for three 377 different time steps in the SUTRA simulation for the hydrostatic 6 m-deep lake scenario: 378 100 years (Figure 8A-B), 240 years (Figure 8C-D), and 1,000 years (Figure 8E-F). 379 Approximate ice-saturation values, translated from the ice versus resistivity relationships 380 for each lithology shown in Figure 2, are displayed on the right axis of each panel in 381 Figure 8, and true resistivity values are plotted as a dashed line. Observations from 382 Figure 8 include: 383 (1) Outside the lake boundary, pdfs are significantly more sharply peaked (darker 384 shading) for the gravel unit than the silt unit, suggesting better resolution of shallower 385 resistivity values within the gravel layer. It should be noted however, that this improved 386 resolution does not imply improved model accuracy; in fact, the highest probability 387 region slightly underestimates the true resistivity value. (2) Probability distributions for 388 the silt layer track the true values, but with greater uncertainty. (3) Inside the lake 389 boundary, gravel resistivity values are not as well resolved compared with locations 390 outside the lake boundary due to the loss of signal associated with the relatively 391 conductive lake water. (4) Increasing trends in resistivity/ice saturation towards the outer 392 extents of the lake are captured in the pdfs, but are subtle. (5) Within the silt layer at 393 early times before the talik is fully through-going (Figure 8B, D), the AEM data are 394 insensitive to which layer is present, hence the bi-modal resistivity distribution with 395 peaks associated with characteristic silt and gravel values. This ambiguity disappears at

396 later times when the low-resistivity unfrozen silt layer extends to the base of the unfrozen 397 gravels, which is a more resolvable target (Figure 8F). 398 A more detailed analysis of the changes in resistivity and ice-saturation as a function of 399 time, and for the differences between hydrostatic and gaining lake conditions, is 400 presented in Figure 9. Average values of resistivity/ice-saturation within 100 m of the 401 lake center are shown within the gravel layer at a depth of 15 m (Figure 9A) and a depth 402 of 50 m within the silt layer (Figure 9B) at 20 year time intervals. Outputs are displayed 403 for both 6 m-deep hydrostatic and gaining lake scenarios. Thawing due to conduction 404 occurs over the first ~200 years within the gravel layer (Figure 9A), with similar trends 405 for both the hydrostatic and gaining lake conditions and no clear relationship to the talik 406 formation times indicated as vertical lines. Conduction-dominated thaw is observed for 407 the gravel layer in the gaining lake scenario because significant advection does not occur 408 until after the thaw bulb has extended beneath the gravel layer. In the deeper silt layer 409 (Figure 9B), however, very different trends are observed for the hydrostatic and gaining 410 lake conditions. Ice content decreases gradually as thawing occurs in the hydrostatic 411 scenario, consistent with conduction-dominated thaw, reaching a minimum near the time 412 of talik formation at 687 years (Wellman et al., 2013, Table 3). In contrast, there is a 413 rapid loss in ice content in the gaining lake scenario resulting from the influence of 414 advective heat transport as groundwater is able to move upwards through the evolving 415 talik beneath the lake. This rapid loss in ice content begins after the gravel layer thaws, 416 and reaches a minimum near the 258-year time of talik formation for this scenario. These 417 trends, captured by the AEM-derived resistivity models, are consistent with the plots of 418 change in ice volume output from the SUTRA simulations reported by Wellman et al. 419 (2013, Figure 3). 420 3.3 **Near-Surface Resolution** 421 Finally, we focus on the upper sand layer (Unit 1), which is generally too thin (2 m) and 422 resistive (> 600 ohm-m) to be resolved using AEM data; though may be imaged using 423 other ground-based electrical or electromagnetic geophysical methods. Seasonal thaw

and surface runoff causes locally reduced resistivity values in the upper 1 m, which is still

too shallow to resolve adequately using AEM data. In practice, shallow thaw and

sporadic permafrost trends are observed to greater depths in many locations, including

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427 inactive or abandoned channels (Jepsen et al., 2013b). To simulate these types of 428 features, the shallow resistivity structure of the 6 m-deep hydrostatic lake scenario at 429 1,000 years is manually modified to include three synthetic 'channels'. These channels 430 are not intended to represent realistic pathways relative to the lake and the hydrologic 431 simulations; they are solely for the purpose of illustrating the ability to resolve shallow 432 resistivity features. 433 Figure 10A shows the three channels in a zoomed-in view of the uppermost portion of the 434 model outside the lake extent. Each channel is 100 m wide, but with different depths: 1 435 m (half the Unit 1 thickness), 2 m (full Unit 1 thickness) and 3 m (extending into the top 436 of Unit 2). Analysis of AEM data simulated for this model, presented as the McMC 437 average model, are shown in Figure 10B. All three channels are clearly identified, but 438 their thicknesses and resistivity values are overestimated and cannot be distinguished 439 from one another. To explore the possibility of better resolving these shallow features, 440 synthetic EM data are simulated using the characteristics of a ground-based multi-441 frequency EM tool (the GEM-2 instrument) that can be hand carried or towed behind a 442 vehicle, and is commonly used for shallow investigations. The McMC average model 443 result for the simulated shallow EM data is shown in Figure 10C. An error model with 444 4% relative data errors and an absolute error floor of 75 ppm was used for the GEM-2 445 data. Channel thicknesses and resistivity values are better resolved compared with the 446 AEM result, though the 1 m-deep channel near r = 800 m appears both too thick and too 447 resistive. In addition, the shallow EM data show some sensitivity to the interface at 2-m 448 depth between frozen silty sands and frozen gravels, though the depth of this interface is 449 over-estimated due to the limited sensitivity to these very resistive features. 450 4 Discussion 451 Understanding the hydrogeophysical responses to permafrost dynamics under different 452 hydrologic and climatic conditions, and in different geological settings, is important for 453 guiding the interpretation of existing geophysical datasets and also for planning future 454 surveys. Geophysical models are inherently uncertain and ambiguous because of (1) the 455 resolution limitations of any geophysical method and (2) the weak or non-unique 456 relationship between hydrologic properties and geophysical properties. We have 457 presented a general framework for coupling airborne and ground-based electromagnetic

458 predictions to hydrologic simulations of permafrost evolution, including a novel physical 459 property relationship that accounts for the electrical response to changes in lithology, 460 temperature, and ice content, as well as a rigorous analysis of geophysical parameter 461 uncertainty. Although the focus here is on AEM data, other types of electrical or 462 electromagnetic measurements could be readily simulated using the same resistivity 463 model. Future efforts will focus on the simulation of other types of geophysical data (e.g. 464 nuclear magnetic resonance or ground penetrating radar) using the same basic modeling 465 approach. 466 In the specific examples of lake talik evolution presented here, which are modeled after 467 the physical setting of the Yukon Flats, Alaska (Minsley et al., 2012), AEM data are 468 shown to be generally capable of resolving large-scale permafrost and geological features 469 (Figure 5), as well as thermally and hydrologically induced changes in permafrost (Figure 470 **8**, Figure **9**). The Bayesian McMC analysis provides useful details about model 471 resolution and uncertainty that cannot be assessed using traditional inversion methods 472 that produce a single 'best' model. A fortuitous aspect of the Yukon Flats model is the 473 fact that the silt layer (Unit 3) is relatively conductive compared with the overlying 474 gravels (Unit 2), making it a good target for electromagnetic methods. If the order of 475 these layers were reversed, if the base of permafrost were hosted in a relatively resistive 476 lithology, or if the base of permafrost was significantly deeper, AEM data would not 477 likely resolve the overall structure with such good fidelity. In addition, knowledge of the 478 stratigraphy helps to remove the ambiguity between unfrozen gravels and frozen silts, 479 which have similar intermediate resistivity values (Figure 4, Figure 5). The methods 480 developed here that use a physical property model to link hydrologic and geophysical 481 properties provide the necessary framework to test other more challenging 482 hydrogeological scenarios. 483 Two key challenges for the lake talk scenarios were identified: (1) resolving the details 484 of partial ice saturation beneath the lake during talik formation, and (2) resolving near-485 surface details associated with shallow thaw. The first challenge is confirmed by Figure 486 5 and Figure 8, which show that AEM data cannot resolve the details of partial ice 487 saturation beneath a forming talik. However, there is clearly a change in the overall 488 characteristics of the sub-lake resistivity structure as thaw increases (Figure 9). One

notable feature is the steadily decreasing depth to the top of the low-resistivity unfrozen silt (red) beneath the lake (Figure 5A-B) as thaw increases, ultimately terminating at the depth of the gravel-silt interface when fully unfrozen conditions exist (Figure 5C). Measurements of the difference in elevation between the interpreted top of unfrozen silt and the base of nearby frozen gravels were used by Jepsen et al. (2013a) to classify whether or not fully thawed conditions existed beneath lakes in the Yukon Flats AEM survey described by Minsley et al. (2012). The simulations presented here support use of this metric to distinguish full versus partial thaw beneath lakes. However, without the presence of a lithological boundary, the shallowing base of permafrost associated with talik development beneath lakes would be much more difficult to distinguish. Finally, it is important to note that resistivity is sensitive primarily to unfrozen water content, and that significant unfrozen water can remain in relatively warm permafrost that is near 0 C, particularly in fine-grained sediments. Resistivity-derived estimates of talik boundaries defined by water content may therefore differ from the thermal boundary defined at 0 C. The second challenge, to resolve near-surface details associated with supra-permafrost thaw, is addressed in Figure 10. For the scenarios considered here, AEM data can identify shallow thaw features, but have difficulty in discriminating their specific details. There are many combinations of resistivity and thickness that produce the same EM response; therefore, without additional information it is not possible to uniquely characterize both thaw depth and resistivity. Ground-based EM data show improved sensitivity to the shallow channels, and also limited sensitivity to the interface between resistive frozen gravels and frozen silty sands (Figure 5). By restricting the possible values of resistivity and/or thickness for one or more layers based on prior assumptions. Dafflon et al. (2013) showed that improved estimates of active layer and permafrost properties can be obtained. The quality of these estimates, of course, depends on the accuracy of prior constraints used. In many instances, it may be possible to auger into this shallow layer to provide direct observations that can be used as constraints. This approach could be readily applied to the ensemble of McMC models. For example, if the resistivity of the channels in Figure 10A were known, the thickness of the channels could be estimated more accurately by selecting only the set of McMC models with channel

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equivalences between layer resistivity and thickness.

AEM data are most likely to be useful for baseline characterization of subsurface properties as opposed to monitoring changes in permafrost. Although there are some cases of rapid change associated with near-surface freeze/thaw processes (Koch et al., 2013) or in the case of catastrophic loss of ice in the gaining lake scenario (Figure 9B) that may be of interest, large-scale changes in permafrost generally occur over much longer time periods than is practical for repeat AEM surveys. One exception could be related to infrastructure projects such as water reservoirs or mine tailing impoundments behind dams, where AEM could be useful for baseline characterization and repeat monitoring of the impact caused by human-induced permafrost change. Geophysical modeling, thermophysical hydrologic modeling, and field observations create a synergy that provides greater insight than any individual approach, and can be useful for future characterization of coupled permafrost and hydrologic processes.

resistivity close to the true value, thereby removing some of the ambiguity due to

5 Summary

Analysis of AEM surveys provide a means for remotely detecting subsurface electrical resistivity associated with the co-evolution of permafrost and hydrologic systems over areas relevant to catchment-scale and larger processes. Coupled hydrogeophysical simulations using a novel physical property relationship that accounts for the effects of lithology, ice saturation, and temperature on electrical resistivity provide a systematic framework for exploring the geophysical response to various scenarios of permafrost evolution under different hydrological forcing. This modeling approach provides a means of robustly testing the interpretation of AEM data given the paucity of deep boreholes and other ground truth data that are needed to characterize subsurface permafrost. A robust uncertainty analysis of the geophysical simulations provides important new quantitative information about the types of features that can be resolved using AEM data given the inherent resolution limitations of geophysical measurements and ambiguities in the physical property relationships. In the scenarios considered here, we have shown that large-scale geologic and permafrost structure is accurately estimated. Sublacustrine thaw can also be identified, but the specific geometry of partial ice

549 saturation beneath lakes can be poorly resolved by AEM data. Understanding the 550 geophysical response to known simulations is helpful both for guiding the interpretation 551 of existing AEM data, and also to plan future surveys and other ground-based data 552 acquisition efforts. 553 **Author contribution** 554 B. M. carried out the geophysical forward and inverse simulations, and prepared the 555 manuscript with contributions from all co-authors. T. W. and M. W. provided SUTRA 556 simulation results and hydrologic modeling expertise. A. R. helped to establish the 557 petrophysical relationships used to define the electrical resistivity model used in this 558 study. 559 Acknowledgements 560 This work was supported by the Strategic Environmental Research and 561 Development Program (SERDP), through grant #RC-2111. We gratefully 562 acknowledge additional support from the USGS National Research Program and the 563 USGS Geophysical Methods Development Project. USGS reviews provided by Josh 564 Koch and Marty Briggs have greatly improved this manuscript. 565

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Tables

Table 1. Description of geologic units and physical properties used in numerical
 simulations. Entries separated by commas represent parameters with different values for
 each of the lithologic units.

Geologic unit properties				
Lithology:				
Unit 1	Sediment (silty sand)			
Unit 2	Sediment (gravelly sand)			
Unit 3	Lacustrine silt			
Unit depth range [m]	0-2, 2-30, 30-250			
Porosity [-]	0.25, 0.25, 0.20			
Geophysical parameters				
Archie cementation exponent (m) [-]	1.5			
Archie saturation exponent (n) [-]	1.5			
Water salinity (C) [ppm]	$250 (S_i = 0)$			
Na ⁺ ionic mobility (β) [m ² /Vs]	5.8 x 10 ⁻⁸ (25°C)			
Cl ⁻ ionic mobility (β) [m ² /Vs]	7.9 x 10 ⁻⁸ (25°C)			
Na^{+} surface ionic mobility (β_s) [m^2/Vs]	0.51 x 10 ⁻⁸ (25°C)			
Grain mass density (ρ _g) [kg/m ³]	2650			
Cation exchange capacity (χ) [C/kg]	200, 10, 500			
Salinity exponent (a) [-]	0.8			

Table 2. Probability of ice saturation falling above or below specified thresholds based
 on the McMC-derived resistivity probability distributions shown in Figure 7.

	p(ice < 0.5)	p(ice > 0.95)
Unit 2 (gravel), $r = 0$ m	0.76	0.05
Unit 2 (gravel), <i>r</i> = 750 m	0.00	0.88
Unit 3 (silt), $r = 0$ m	0.76	0.05
Unit 3 (silt), r = 750 m	0.00	0.98

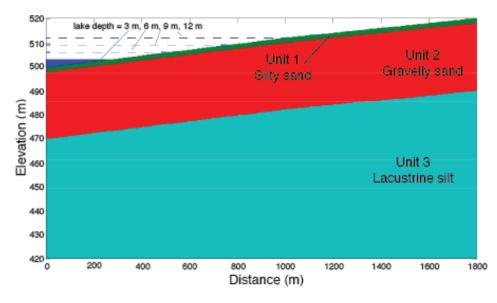


Figure 1. Axis-symmetric model geometry indicating different lithologic units and simulated lake depths/extents.

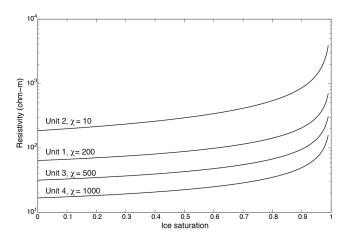


Figure 2. Bulk resistivity as a function of ice saturation using the physical properties defined for each of the lithologic units described in Table 1.



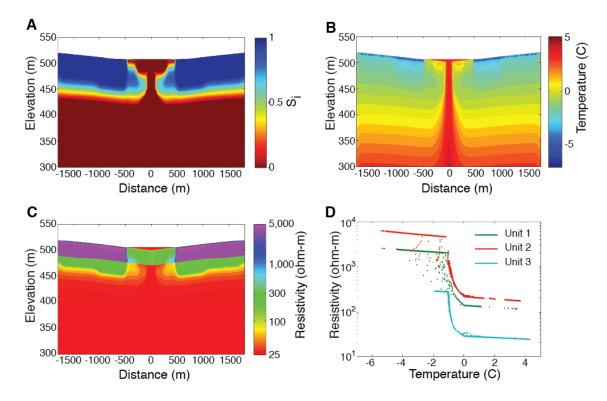


Figure 3. SUTRA model outputs and geophysical transformations from the 6-m gaining lake simulation at 240 years. Ice saturation (A) and temperature (B) are converted to predictions of bulk resistivity (C). Variability in resistivity as a function of temperature is indicated in (D) for lithologic units 1-3.

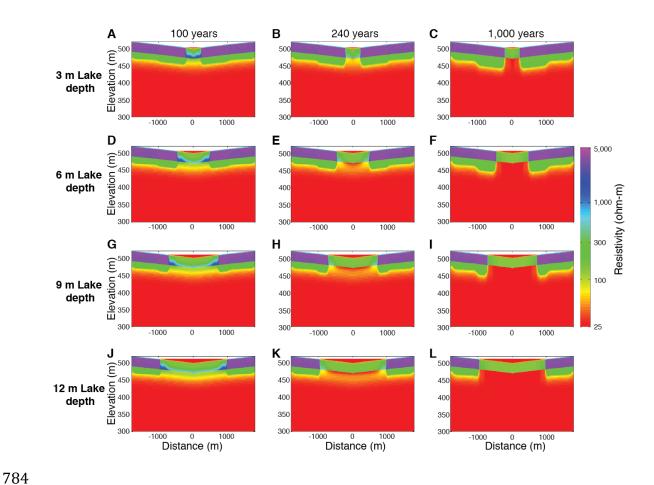


Figure 4. Synthetic bulk resistivity images under hydrostatic flow and current climate conditions. Lake depths of 3 m (A-C), 6 m (D-F), 9 m (G-I), and 12 m (J-L) are illustrated at simulation times 100, 240, and 1,000 years.

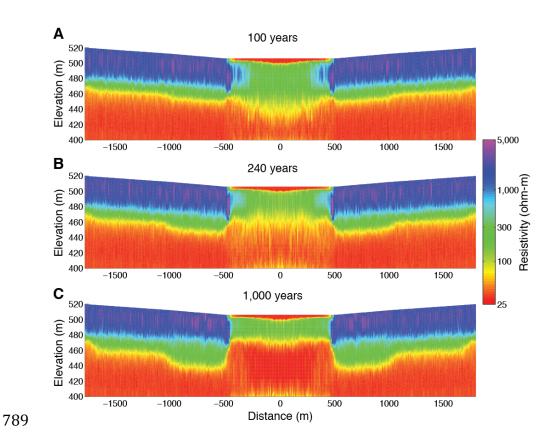


Figure 5. Mean resistivity model extracted from McMC ensembles. Results are shown for the 6-m-deep hydrostatic lake scenario outputs at (A) 100 years, (B) 240 years, and (C) 1,000 years.

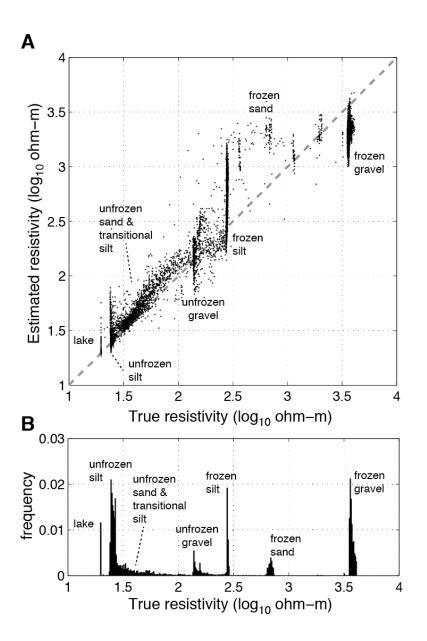


Figure 6. Performance of geophysical parameter estimation in recovering true parameter values. (A) True versus McMC-estimated resistivity values for the hydrostatic 6-m-deep lake scenario at simulation time 1,000 years, compared with the frequency distribution of true resistivity values (B). Estimated resistivity values generally fall along the dashed 1:1 line in (A), with exceptions being under-prediction of the resistive frozen gravels, overprediction of the thin surficial frozen sand, and some over-prediction of the frozen silt where it is in contact with frozen gravel.

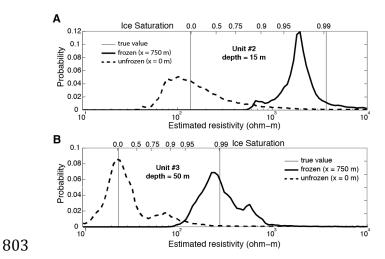


Figure 7. McMC-estimated resistivity posterior distributions within frozen and unfrozen unit #2 gravels (A) and frozen and unfrozen unit #3 silts (B) for the hydrostatic 6-m-deep lake scenario at 1,000 years. Unfrozen resistivity distributions are extracted beneath the center of the lake (r = 0) at depths of 15 m and 50 m for the gravels and silts, respectively. Frozen distributions are extracted at the same depths, but at r = 750 m. The upper x-axes labels indicate approximate ice saturation based on the lithology-dependent ice saturation versus resistivity curves shown in Figure 2.

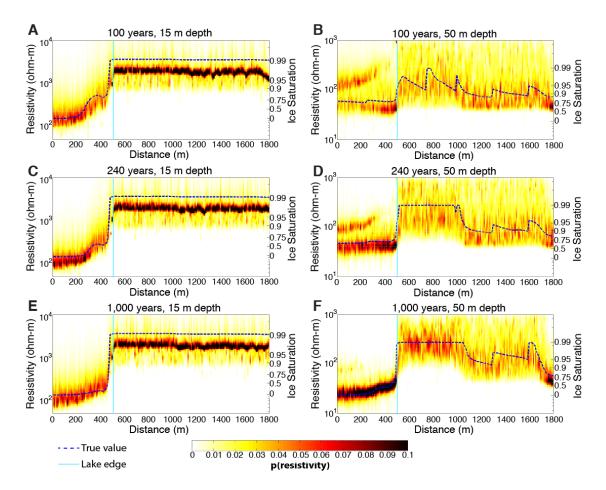


Figure 8. Resistivity probability distributions for the hydrostatic 6-m-deep lake scenario at simulation times 100 years (A-B), 240 years (C-D), and 1,000 years (E-F). Shading in each image represents the probability distribution at depths of 15 m (A, C, E) and 50 m (B, D, F) from the lake center (r = 0 m) to the edge of the model (r = 1800 m). Dashed lines indicate the true resistivity values. Ice saturation is displayed on the right axis of each image, and is defined empirically for each lithology using the relationships in Figure 2.

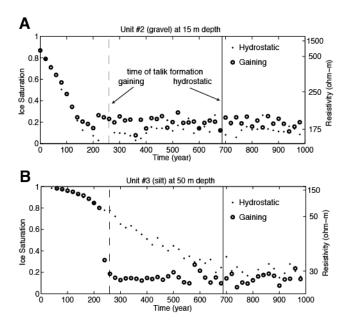


Figure 9. Change in ice saturation and resistivity as a function of time. Results are shown for the 6-m-deep lake hydrostatic and gaining lake scenarios within (A) the gravel layer, unit #2, at a depth of 15 m and (B) the silt layer, unit #3, at a depth of 50 m.

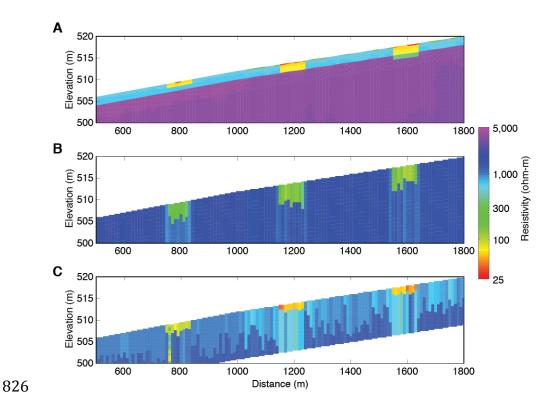


Figure 10. Comparison of airborne and ground-based measurements for recovering shallow thaw features. (A) True shallow resistivity structure extracted from the hydrostatic 6-m-deep lake scenario at a simulation time of 1,000 years, shown outside of the lake extent (distance > 500 m). Three shallow low-resistivity channels with thicknesses 1 m, 2 m, and 3 m were added to the resistivity model to provide added contrast. McMC-derived results using simulated AEM data (B) and ground-based EM data (C) illustrate the capability of these systems to image shallow features.