

Modeling different freeze/thaw processes in heterogeneous landscapes of the Arctic polygonal tundra using an ecosystem model

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Abstract

Freeze/thaw (F/T) processes can be quite different under the various land surface types found in the heterogeneous polygonal tundra of the Arctic. Proper simulation of these different processes is essential for accurate prediction of the release of greenhouse gases under a warming climate scenario. In this study, we have incorporated the water layer into a dynamic organic soil version of the Terrestrial Ecosystem Model (DOS-TEM), having—We first verified and validated the DOS-TEM model. Results showed that: (1) the DOS-TEM was very efficient and its results compared very well with analytical solutions for idealized cases, and; (2) although there were despite a number of model—limitations and uncertainties in the modeling, the simulations compared reasonably well with *in situ* measurements ~~on from the~~ polygon rims, polygon centers (with and without water), and lakes on the Samoylov Island, Siberia. Therefore, wWe concluded that the DOS-TEM is suitable ~~tefor~~ simulating these different various F/T processes. We then performed sSensitivity tests were then performed on the effects of water depth. Our results indicated, that [water], in addition to as well as snow cover, is very important in the simulated thermal processes for both polygonal centerres and lakes types. Therefore, We therefore concluded that the polygonal rims and; polygonal centers (with various maximum water depths) should be considered separately, ÷ and that the dynamics of water depth ~~of in~~ both polygonals and lakes should also be ~~considered taken into account~~ when simulating thermal processes for methane emission studies. We then performed sensitivity tests on the effects of water depth. Our results indicate that water is very important in the simulated thermal processes, which are especially sensitive to changes of water depth when it is between 1 and 2m. Therefore, we conclude that the land surface without water (rim and center without standing water), polygonal center with water (with various depths) and lake (with various depths) should be considered separately when simulating thermal processes for methane emission studies; and the DOS-TEM is suitable to simulate these different F/T processes. In this study we have modified the dynamic organic soil version of the Terrestrial Ecosystem Model (DOS-TEM) to simulate F/T processes beneath the polygon rims, polygon centers (with and without water), and lakes that are common features in Arctic lowland regions. We first verified the F/T algorithm in the DOS-TEM against analytical solutions, and then compared the results with *in situ* measurements from Samoylov Island, Siberia. In the final stage, we examined the different responses of the F/T processes for different water levels at the various land surface types. The simulations revealed that (1) the DOS-TEM was very efficient and its results compared very well with analytical solutions for idealized cases, (2)

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~~the simulations compared reasonably well with in situ measurements although there were a number of model limitations and uncertainties, (3) the DOS-TEM was able to successfully simulate the differences in F/T dynamics under different land surface types, and (4) permafrost beneath water bodies was found to respond highly sensitive to changes in water depths between 1 and 2 m. Our results indicate that water is very important in the thermal processes simulated by the DOS-TEM; the heterogeneous nature of the landscape and different water depths therefore need to be taken into account when simulating methane emission responses to a warming climate.~~

1 Introduction

The release of greenhouse gases from the large quantities of soil carbon preserved in Arctic regions constitutes an important feedback to climatic warming and the thawing of permafrost north of 45°N (McGuire et al., 2009; von Deimling et al., 2012). Reliable simulation of the dynamics of permafrost is therefore critical when predicting future climatic changes. The energy balance ~~of at the~~ ground surface has an important influence on variations in permafrost. Heterogeneous ground surfaces with ~~(e.g., variable snow pack thicknesses and organic layer thicknesses)~~, ~~have exert~~ a ~~large-major~~ influence ~~on~~ the ~~on~~-surface energy balance (Eitzelmüller and Frauenfeld, 2009); and have in the past been integrated into both land surface models (Yi et al., 2007; Lawrence and Slater, 2008) and ecosystem models (Zhuang et al., 2001; Yi et al., 2009a,b; Yi et al., 2010). ~~However, few of the current large scale land surface models or ecosystem models take into account the effects that water bodies have on the dynamics of permafrost (Zhuang et al., 2006; Ringeval et al., 2012), with one exception being the model by Wania et al. (2009) which treated surface water in the same way as a litter layer.~~ Water bodies of various sizes, ranging from those occupying polygon centers to large thermokarst lakes, are distributed across the Arctic coastal regions (French, 2007) resulting in considerable landscape heterogeneity. Water bodies ~~strongly have a marked æ~~effect ~~on~~ the surface energy balance and ~~the~~ thermal dynamics of the surrounding permafrost soils (French, 2007). Their presence can lead to permafrost degradation, which in turn affects the terrestrial ecosystem's carbon budget. ~~For example, Q~~outgassing of carbon dioxide from ponds and lakes was, ~~for example, found-calculated~~ to account for between 74 and 81% of the ~~calculated~~ net landscape-scale CO₂ emissions ~~in polygonal tundra in the Lena Delta (Siberia) during September~~ (Abnizova et al., 2012). ~~However, few of the current large scale land surface models or ecosystem models take into account the effects that water bodies have on the~~

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dynamics of permafrost (Zhuang et al., 2006; Ringeval et al., 2012), with one exception being the model by Wania et al. (2009) which treated surface water in the same way as a litter layer.

There are a number of different techniques ~~for used to~~ simulate permafrost dynamics (Riseborough et al., 2008). A wide range of numerical models exist, which are applied ~~in~~ both in stand-alone permafrost simulations and in land-surface schemes of climate models. Soil ~~The~~ temperatures and water content at different depths ~~of in~~ soil or rock are calculated numerically. ~~In large scale models~~ Numerical solutions ~~of for~~ permafrost dynamics in large scale models are commonly obtained by solving finite difference equations. One category of numerical solution, referred to by Zhang et al. (2008) as "decoupled energy conservation parameterization", assumes that the soil water is homogeneous and freezes or thaws at exactly 0°C. Soil temperature is calculated for each layer and; ~~if following calculation of the soil temperature for each layer~~ the temperature of a particular layer ~~that contains ice~~ is then greater than 0°C, some or all of any present ~~the~~ ice will melt and the temperature is then recalculated, and *vice versa*. This is an efficient method and is commonly used in land surface models (Zhang et al., 2003; Oleson et al., 2004). However, the lower layers in land surface models are usually thick and the ~~derived~~ freezing or thawing fronts derived from soil temperature interpolation are not realistic (Yi et al., 2006).

A second category of numerical methods, referred to by Zhang et al. (2008) as "apparent heat capacity parameterization", assumes that soil water freezes or thaws over a range of temperatures below 0°C and simulates the unfrozen soil water content and temperature simultaneously. Since small changes ~~of in~~ soil temperature within the freeze/thaw range will result in a large change in apparent heat capacity, an iterative procedure is required to ensure that only small temperatures ~~changes of temperature at during~~ each time interval (Nicolsky et al., 2007). This method is commonly applied in permafrost models (Goodrich, 1978; Nicolsky et al., 2007; Dall'Amico et al., 2011; Hipp et al., 2012; Langer et al., 2013) and has also recently been applied in a land surface model (Ringeval et al., 2012). Although the method is more physically realistic it requires greater computing resources. This may lead to limitations in the spatial resolution, the length of time that can be modeled, and the number of simulated land surface classes, etc.

Both categories of numerical models have their disadvantages when they are applied for regional permafrost simulation. ~~Besides~~ Apart from numerical models, analytical solutions also exist that can be used for solving phase change problems. For example, exact Neumann solutions to freezing and thawing problems exist for idealized cases, e.g. for infinite or semi-

infinite homogeneous material, steady upper boundary conditions, etc. (Lunardini, 1981). Stefan's equation, which was originally used to predict the thickness of sea ice, is widely used due to its simple form (Lunardini, 1981); an algorithm for applying Stefan's equation to a layered system (e.g. soil) was developed by Jumikis (1977) and applied in a hydrological model by Fox (1992). However, predictions from the Stefan algorithm usually overestimate the depths of freeze/thaw fronts as it neglects any heat transport ~~below-beneath the front-is neglected~~. In order to mitigate this problem of overestimation, Woo et al. (2004) developed a two-directional Stefan algorithm (TDSA). Yi et al. (2009a) integrated a TDSA within a Terrestrial Ecosystem Model (TEM) in order to first simulate the depths of freezing or thawing fronts, and then update the soil temperatures for layers above the uppermost front, ~~below-beneath~~ the lower-most front, and between these two fronts. This is an efficient method and is able to track the positions of fronts within thick soil layers.

Although models using the above methods to simulate permafrost dynamics over large regions have been validated using in situ measurements, few of them have been verified against analytical solutions for both freeze~~e~~~~ing and~~ thaw~~ing~~ fronts and soil temperatures at different depths, which is as important as-for model validation (Romanovsky et al., 1997). Furthermore, conceptual and numerical permafrost landscape models also require suitable upscaling methods ranging from local to global scales, based on field-based knowledge of the surface characteristics, key processes and data collection of key parameters (Boike et al. 2012).

In this study we aimed to develop and test a model that could simulate permafrost dynamics under different types of land surface, i.e. different thicknesses of snow cover, of the organic layer, and of ~~of~~ water cover. We first verified our dynamic organic soil version of the TEM (DOS-TEM), which used the TDSA to simulate soil freezing/thawing processes, with analytical solutions for idealized cases. ~~we~~ We then modified the model to take into account the effects that water bodies of various sizes have on the thermal dynamics of permafrost and compared the output with in situ measurements from Samoylov Island ~~in the Lena Delta~~, Siberia. Finally, we compared the simulations ~~under-beneath~~ different land surface types in order to investigate the vulnerability~~ies~~ of permafrost to water bodies.

2 Methods

2.1 Site description

Samoylov Island (72°22'N, 126°30'E) is located in the southern-central part of the Lena River

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Delta of Siberia (Figure 1); it covers an area of about 4.37-5 km². The average annual mean air temperature on Samoylov Island from 1998 to 2011 was -12.5°C and the average total summer rainfall 125 mm (Boike et al., 2013). Samoylov Island contains two major geomorphological units: a floodplain, and an elevated Holocene terrace ~~which-that~~ is characterized by low-centered polygonal tundra. The elevated terrace comprises ~70% of the total area of the island and contains numerous ponds and thermokarst lakes. On average, the land surface of the terrace consists of 58% dry tundra, 17% wet tundra, and 25% water surfaces (Muster et al., 2012). A 26.75 m borehole was drilled in 2006. It is located in an area that consists of about 60% of polygonal centeres and of about 40% of polygonal rims, with a negligible area. The areal fractionl proportion of ponds in the vicinity of the borehole is negligible (Figure 1). Further information concerning the climate, permafrost, vegetation, and soil characteristics can be found in Boike et al. (2013).

2.1.1 Meteorological data processing

The collection of meteorological measurements on Samoylov Island started in 1998. The daily mean air temperature, wind speed, vapor pressure, net radiation, downward solar radiation, and total daily precipitation were calculated from hourly measurements. If more than 25% of the measurements were missing in any one day, no value was recorded for that day. If more than 25% of the daily values in a particular month were missing, no value was recorded for that month. We replaced the missing monthly values as follows:

- (1) Air temperature and precipitation (snow + rain) measurements for the same month, available from the nearby Stolb meteorological station (which has datasets from 1956, but with large gaps during the 1970s), were used to replace the missing values.
- (2) Long term-mean values were used to replace some values for air temperature and precipitation that remained missing after step (1) above, as well as missing values for wind speed, radiation, and vapor pressure. We calculated the long-term monthly mean for air temperature and precipitation between 1981 and 2011 using measurements from the Stolb meteorological station, and for wind speed, downward shortwave radiation, and vapor pressure between 1998 and 2011 using measurements from the Samoylov site.

To illustrate the differences between different datasets, we compared the monthly air temperature and precipitation datasets from Samoylov Island with those from Stolb and the global reanalysis dataset from the Climate Research Unit (CRU TS3.1), available from

http://badc.nerc.ac.uk/view/badc.nerc.ac.uk_ATOM_dataent_1256223773328276 (Figure 2).

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2.2 Model descriptions

The Terrestrial Ecosystem Model (TEM) family of models is designed to simulate the carbon and nitrogen pools within vegetation and soil, and the carbon and nitrogen fluxes between vegetation, soil, and the atmosphere (McGuire et al., 1992). The most recent TEM version (i.e. the DOS-TEM) can simulate the dynamics of organic soil layers, which can be subject to fire disturbances and to ecological successions (Yi et al., 2010). The DOS-TEM consists of four modules, these being the environmental, ecological, fire disturbance, and dynamic organic soil modules. The environmental module operates on a daily time interval using mean daily air temperature, surface solar radiation, precipitation, and vapor pressure, which are downscaled from monthly input data (Yi et al., 2009a). It takes into account radiation and water fluxes between the atmosphere, canopy, snow pack, and soil. Soil moisture and temperature of all soil layers are updated daily. A two-directional Stefan algorithm is used to predict the depths of freezing or thawing fronts within the soil (Woo et al., 2004); it first simulates the depth of the front in the soil column from the top downward, using soil surface temperature as the driving temperature; it then simulates the front from the bottom upward using the soil temperature at a specified depth beneath a front as the driving temperature (bottom-up forcing). If a layer contains a freezing or thawing front, this layer is then divided into two layers (Figure A1b). The temperatures of soil layers above the uppermost freezing or thawing front and ~~below~~ beneath the lowermost freezing or thawing front are updated separately by solving finite difference equations. The thermal properties of soil layers are affected by their water content (Yi et al., 2009a).

2.3 Model modifications

We made three modifications to the DOS-TEM in order to simulate the effects that water bodies (Figure A1a) have on freezing or thawing processes. (1) As shown in Figure A3a, the volumetric water content of a polygon at center is not equal to 1, due to the soil surrounding water bodies. We took into account ~~the this effect of the soil surrounding water bodies~~ by calculating the volumetric water content of different layers within water bodies of various sizes (Figure ~~A2~~ A3); details are presented in Appendix ~~AB~~. (2) When updating the thermal state of water layers they were treated in the same way as soil layers, but with different thermal properties. We followed the model of Hostetler et al. (1990) to calculate the eddy

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diffusion coefficients for the water layers, which were then used, together with the molecular diffusion coefficient of water, to calculate the heat transfer within the water bodies and the heat exchange with the underlying sediments. Details are presented in Appendix B. (3) The original DOS-TEM only simulated bottom-up forcing for the deepest freezing or thawing front. However, taliks probably exist beneath some water bodies, and more than ~~2~~ two freezing or thawing fronts may exist at the same time. We therefore implemented top-down and bottom-up forcing separately for each front (~~Figure A1b~~ Appendix A).

The soil thermal conductivity in the DOS-TEM was initially calculated according to Farouki (1986). However, preliminary testing showed that the ~~calculated~~ resulting soil thermal conductivities were higher than those derived from field measurements (Langer, et al., 2011 a and b). ~~Hence, in this study w~~ We therefore used the more realistic parameterization according to Johansen (1975) and Côté and Konrad (2005). ~~More~~ Further details on the ~~used~~ parameterization used are provided in Appendix ~~BC~~.

2.4 Model verification, validation and sensitivity tests

2.4.1 Comparisons with analytical solutions

Three different materials were tested in this study, i.e. water, minerals (sand), and organic soil. The properties of these materials are listed in Table 1. The initial temperature of each material at different depths (up to 5000 m in the DOS-TEM) was set to -10°C , and the temperature at the upper boundary of each material was set to 5°C over the whole simulation period (100 yrs). We assumed zero heat flux conditions at the lower boundary, ~~i.e. in at~~ 5000 m depth. The temperatures and the depth of the thawing front obtained from the DOS-TEM were compared with those from analytical solutions and those obtained using the one-directional Stefan's equation. For the DOS-TEM, the temperature at a specific depth was calculated by linear interpolation between the temperatures of ~~upper overlying~~ and ~~lower underlying~~ layers. To test the sensitivity of the model to the depth used for the bottom-up forcing, we tried bottom-up forcing at different depths below the thawing front (i.e. at 50 cm, 1 m, 2 m, 5 m, and 20 m ~~below~~). In order to test the effects of total soil/water thickness, we also evaluated the DOS-TEM ~~for using~~ different depths ~~of for the~~ lower boundary (50, 500, and 5000 m). The maximal thicknesses of the soil/water layer ~~were was set to~~ 1 m, 10 m, and 100 m for ~~the~~ runs with the lower boundary ~~located in at~~ 50 m, 500 m, and 5000 m depth, so that the total number of layers was constant for each run.

2.4.2 Comparisons with *in situ* measurements

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Test sites

We tested the DOS-TEM for soil or water temperatures at 4 different sites, i.e. on a polygon rim (*rim*), in a polygon center without standing water (*center*), in a polygon center with standing water (*pond*), and ~~in a~~ larger thermokarst lake (*lake*). These sites are considered to represent the most ~~prominent~~important types of land surfaces in the polygonal tundra landscape of Samoylov Island. The configurations of ~~the~~ water and organic soil characteristics for the different land surface types used in the model are presented in Table 2. ~~We~~We used about 65 m of mineral soils (saturated sand with a porosity of 0.6) in 12 layers. The DOS-TEM assumes bedrock beneath the soil layer (Figure A1a); in each case we used 420 m of bedrock in 5 layers to represent the frozen sediments on Samoylov Island. The ground heat flux at the bottom of the bedrock was set to 0.053 w/m² (Pollack et al. 1993).

The simulated soil temperatures ~~at for~~ the four different land surface types were compared to temperature measurements from a 27m borehole on Samoylov Island (Boike et al. 2013).

Surface temperatures

The DOS-TEM ~~does not~~is not able to simulate the surface temperatures of water, land, or snow ~~as what land surface model does~~. We therefore used linear regression to established the relationships ~~by linear regression~~ between measured daily surface temperatures and air temperatures ~~in during those periods of 2011, when in which both temperatures are were~~ greater than above 0°C, as follows: for water $T_{surf} = 0.563T_{air} + 4.735$ (coefficient of determination (R^2) = 0.41, number of pairs of data (n) = 84), for land, $T_{surf} = 0.643T_{air} + 2.231$ (R^2 = 0.54, n = 84), ~~and for~~ for snow, frozen soil and frozen water we assumed $T_{surf} = T_{air}$. A similar method has previously been used in Yi et al. (2013).

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Snow cover

Wind drift is an important process that redistributes snow ~~in on~~ the polygonal tundra landscape. Field measurements of annual maximum snow thickness ~~are show depths of~~ usually 15-40 cm in polygon centers and much less on polygon rims ~~(10-30 cm, with the an average at of about 15 cm)~~ and frozen lakes (Boike et al., 2013). Zhang et al. (2012) introduced a snow drift factor into their NEST model. The factors for ~~polygon rims, polygon centers without standing water, and polygon centers with standing water~~ water bodies (ponds and lakes) ~~are were~~ 0.5, 0, and -0.25, respectively, with a positive value indicating a loss of snow due to wind drift. However, a preliminary model run indicated that the simulated snow

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thicknesses were overestimated~~ds~~, for all sites. ~~Therefore, in this study, we therefore identified site-specific threshold values of maximum snow accumulation based on field observations, as follows:~~ Therefore the maximum snow thickness was set to 0.1 m for both polygon rims and lakes. For polygon centers we assumed that

$$D_{snw,max} = \begin{cases} 0.15 & \text{rim} \\ \Delta H + 0.15 & \text{centre} \\ 0.15 & \text{lake} \end{cases}$$

$$D_{snw,max} = (WD_{max} - WD) + 0.1$$

~~W~~ here $D_{snw,max}$ is the maximum snow thickness (m), WD_{max} ~~is~~ ΔH is the maximum water depth/microtopographic relief height (m), and WD is the actual water depth (m) (see Figure A2A3).

We also assumed that snow only accumulates when the top layer of ~~the~~ soil or water is frozen.

Soil and water properties

For the soil thermal properties we used two sets of parameters, one derived from field temperature measurements (Langer et al., 2011a and b) and the other calculated from an algorithm proposed by Luo et al., (2009), details of which can be found in Appendix B-C (Table 3). For water, we increased the calculated value of the eddy diffusion coefficient by a factor of between 10 and 100 (following Subin et al., (2012), in order to take into account the effects of convection currents caused by complex lake topography and density instability.

Initialization

The *rim*, *center*, and *pond* sites were all initialized using a temperature of -10°C for all water, soil, and bedrock layers; the *lake* site was initiated with -10°C for all soil and bedrock layers and with 0°C for water layers. ~~In order to reach realistic temperature distributions within the ground, the model was run to a dynamic equilibrium over a 100-year period at the rim, center, and pond sites and a 200-year period at the lake site.~~ For the equilibrium run, the model was forced by an average annual cycle that was generated ~~from using~~ the monthly averages ~~of generated from the available~~ climate data ~~available from for~~ 1981 to 2011. ~~When the difference of in annual mean unfrozen soil thicknesses of between two consecutive consecutive years is was less than 0.01 cm, the model is was considered to be in a state of equilibrium state.~~ The equilibrium run time was set to ~~be~~ between 50 and 400 yr. The state of equilibrium was verified by additional runs using longer periods of 400 and 600 years respectively. The period

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from 1981 to 2003 was used for model spin-up, and we compared the simulations with measurements collected after 2003.

2.4.3 Effects of (maximum) water depth

Polygon centers and lakes of various sizes and water depths are distributed across much of Samoylov Island. In order to investigate the effect that the size and water depth of polygon ponds and lakes have on the thickness of the underlying unfrozen soil ~~underneath~~, we ran the DOS-TEM for a shallow, medium, and deep polygon pond (with maximum water depths of 20, 60, and 120 cm), and for a shallow, medium, and deep lake (with maximum water depths of ~~32, 64, and 96~~ m). For each polygon pond or lake the model was run with water depths of between no water (empty), with 50% (half full), and 100% (full) of to 0 and 100% of the maximum water depth, at an intervals of equal to 5% of the maximum water depth. The annual mean unfrozen soil thickness ~~of each run~~ from ~~1981-2003~~ to 2011 was calculated for each run, for comparison purposes.

3 Results

3.1 Comparisons with exact Neumann solutions and Stefan equations

The bottom-up forcing in the DOS-TEM is very important for accurate simulation of the position of the thawing front using Stefan's algorithm (Figure 3). For all cases of water, mineral soil, and organic soil, the thawing fronts simulated without bottom-up forcing were very close to those calculated using Stefan's equation. The root mean squared errors (RMSEs, $n = 36,500$) between ~~simulated~~ thawing fronts simulated without bottom-up forcing and those from exact Neumann solutions for three different idealized cases were greater than 1.128 m. In contrast, the RMSEs between the ~~simulated~~ thawing fronts simulated with bottom-up forcing and those from exact Neumann solutions were less than 0.047 m (Table 4).

The simulated water or soil temperatures and thawing fronts were not sensitive to the depth of bottom-up forcing (Figure 3). For example, there ~~were was~~ almost no differences ~~in-between~~ the ~~simulated~~ thawing fronts simulated for bottom-up forcing at depths ~~from-of between~~ 0.5 m ~~to-and~~ 20 m, in all three cases (water, mineral soil, and organic soil). The differences between ~~simulations-of-the~~ thawing front simulations using ~~these~~ bottom-up forcing and those from Neumann solutions were also very small (Figure 3). Taking bottom-up forcing at a depth of 1 m beneath the thawing front as an example, most of the RMSEs for temperatures at depths

shallower than 1 m were less than 0.01°C, and approximately 0.1°C for depths greater than 1m (Figure 4 and Table 5).

The simulated temperatures ~~are-were~~ sensitive to the total thicknesses of the various materials, especially ~~for-that-of~~ mineral soil which has the highest thermal conductivity and the lowest water content (Table 4).

3.2 Comparisons with in situ measurements

3.2.1 Snow thicknesses

The simulated snow thickness from the DOS-TEM was ~~more-greater~~ than 80 cm at all sites for 2005-2006, and decreased thereafter (Figure 5). However, measurements at the *center* site showed that the monthly maximum snow thickness was only 40 cm. After setting a maximum snow thickness, the differences in snow thickness between the 4 sites were similar to field observations, but the inter-annual variability was very small. Since we assumed that snow only accumulates on frozen layers of water or soil, the starting date for snow accumulation at *pond* and *lake* sites was usually later than at *rim* and *center* sites. The simulated starting dates for snow accumulation in the autumn of 2010 were about one month later than the observed starting dates.

3.2.2 Temperatures of shallow layers

For the *rim* site, soil temperatures for model runs that included snow drift compared well with actual measurements at depths of both 2 cm and 51 cm- (Figure 6). The simulated soil temperatures at 51 cm were slightly lower than measured temperatures-underestimated during summer months. The simulated soil temperatures using the calculated thermal properties (Appendix BC) were close to those simulated using the derived thermal properties at 2 cm depth but varied by about 1-3°C at 51 cm depth. The effect of snow was very obvious: where no maximum snow thickness had been set the simulated soil temperatures were up to 10°C warmer than the measured soil temperatures.

For the *center* site, the performance of the DOS-TEM was similar to the *rim* site during the summer seasons (Figure 7). The DOS-TEM overestimated the soil temperatures at 40 cm depth in several of the winters. Using different soil thermal properties did not result in any obvious differences in soil temperatures, and setting a maximum snow thickness had less effect than for the *rim* site.

For both *rim* and *center* sites, the simulated soil temperatures fell rapidly during the fall of 2010, possibly due to the later snow fall in the simulation (Figures 5, 6, and 7).

For the *pond* site, ~~the model underestimated water temperatures in summer and overestimated them in winter~~ the amplitude of the seasonal cycle of simulated water temperature was had a reduced amplitude (Figure 8). For example, the simulated water temperature in the lower part of the *pond* site was 20°C warmer than actual measurements from the winter of 2008-2009. As an additional experiment we reduced the maximum snow thickness from 15 cm to 2 cm, which brought the simulated water temperatures in winter down to the measured temperatures. ~~Setting a maximum snow thickness thus reduced the simulated water temperature in winter.~~ Changing the water eddy diffusion coefficient by a factor of between 10 and 100 did not result in any obvious differences between model runs.

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For the *lake* site, the simulated water temperatures in the upper part of the lake were not as sensitive to the eddy diffusion coefficient as those in the lower part of the *lake* (Figure 9). The simulation using the default water eddy diffusion coefficient considerably underestimated the water temperature (by about 10°C) in the lower part of the *lake*. Increasing the eddy diffusion coefficient by a factor of 100 improved the simulation.

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In the following two subsections we only analyze the freezing and thawing fronts and the deeper soil temperatures ~~off from the lake site~~ on the basis of simulations with a maximum snow thickness, derived soil thermal properties, and an eddy diffusion coefficient increased by a factor of 100.

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3.2.3 Freezing and thawing fronts and unfrozen soil thicknesses

The simulated shapes of freezing and thawing fronts at the *rim* and *center* sites were similar from 2003 to 2011 (Figure 10). The thawing fronts did not survive through the winter months and into the following year. However, multiple thawing and freezing fronts were simulated at the pond site. ~~the simulated thawing fronts at the pond site were usually static in summer and autumn, and usually extended through the winter into the following spring.~~ In an additional test performed with 2 cm maximum snow thickness, the soil temperature was colder than it was with ~~15-20~~ cm maximum snow thickness and the shapes of the thawing fronts were

different (Figure 10.3c) and 4d)). However, from 2003 to 2011 the average maximum depth of thawing fronts in soils under water was 0.47 for simulations with 2 cm maximum snow thicknesses and 0.583.86 m for those with 15-20 cm maximum snow thickness. The simulated thawing fronts at the lake site occurred at an average depth of 9.67-12.90 m below the lake floor. We also performed an additional simulation using bottom up forcing only for the deepest thawing front. Results showed only a few centimeters difference between the depths of freezing fronts in lake water from this additional simulation and those from the original simulation (details not included).

The maximum active layer thickness, which is defined as the maximum unfrozen thickness of the active layer over a complete year, varied in 2010 from 0.33 m in 2004 to 0.65 m at the rim site, from 0.34 m in 2004 to 0.57 m at the center site, and from 0.5m to 0.8 m below the floor of the polygon e pond. The DOS-TEM did not simulate any talik for these three sites between 2003 and 2011 but simulated about 9.67 m of talik beneath the lake site.

The volumetric water content (VWC) of polygon centers or lakes was reduced by only 6% less (at the most) with than the bathymetry of the water depths measured on Samoylov Island (Table A1). We investigated the effects of including a VWC calculation by comparing two sets of simulations: one considering taking into account the effects of bathymetry water depth on the VWC, and the other using a VWC= of 1. The differences of multi-year mean simulated unfrozen soil thickness were very small (less than 1 cm) for the lake site and the pond site with 2 cm maximum snow thickness. However, for the comparison at the pond site with 20 cm maximum snow thickness, the simulated unfrozen soil thicknesses for both the two simulations were about 1.60 and 3.66 m, respectively.

In order to investigate the effects of eddy diffusivity and equilibrium run time, we performed additional sensitivity tests at on the lake site, with three different eddy diffusivities (the original value of ke_1 , and additional values of multiplied by 10 (ke_{10}) and 100 (ke_{100})) and 3 equilibrium run times (200, 400, and 600 yr). The simulation with ke_1 and a 200 yr equilibrium run time had the smallest talik thickness (8.42 m), while that with ke_{100} and a 600 yr equilibrium run time had the largest greatest unfrozen soil thickness (16.11 m). For a specified particular equilibrium run time, the effects of that increasing the eddy diffusivity from ke_1 to ke_{10} had on soil-unfrozen soil thickness were greater between ke_1 and ke_{10} than between the effect when it was increases from ke_{10} and to ke_{100} . For a specified particular eddy diffusivity value, the effects of increasing the equilibrium run

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time from 200 to 400 yr ~~werewas~~ similar ~~between 200 and 400 yr as between~~ to that of increasing it from 400 ~~and~~ to 600 yr (Table 6).

Previous versions of the DOS-TEM only considered top-down forcing for the uppermost front and bottom-up forcing for the lowest front. In this study, we implemented both top-down and bottom-up forcings for each front. There were very small differences at the *rim*, *center* and *pond* sites, but ~~prominent~~ major differences at the *lake* site. For example, with eddy diffusivity increased by a factor of 10 ~~times~~ and a 400 yr equilibrium run time, the simulated unfrozen soil thicknesses over the period ~~offrom 2003 to~~ 2011 ~~werewas~~ about 10.96 and 12.89 using our version of the DOS-TEM, compared to 10.96 ~~for~~using the previous ~~and current~~ version (Yi et al., 2009a) ~~s of DOS-TEM, respectively.~~

~~Increasing the equilibrium run time for the lake site, from 200 years to 400 or 600 years increased the multi year mean talik thickness between 2007 and 2011 from 9.67m to 11.46 or 13.60 m, respectively. Hence, no thermal equilibrium was reached at the lake site.~~

3.2.4 Temperatures of deep layers

The averages of the modeled annual mean soil temperatures at 26.75 m depth over the period from 2007 to 2011 were approximately ~~-10.9~~10.16, ~~-9.29~~14, ~~-3.099~~, and ~~-1.20~~61°C for the *rim*, *center*, *pond*, and *lake* sites, respectively (Figure 11). ~~The size of centeres and rims isare typically on the order of about 10 m across— and It can be assumed that horizontal temperature differences due to surface heterogeneities arecan be assumed to be largely averaged out forat depths greater than 10m. Therefore, t~~ The borehole temperatures ~~inat~~ depths ~~larger~~greater than 10 m ~~therefore~~ represent an averages temperature beneath both polygon centers and polygon rimse~~r~~. If the simulated temperatures from the *rim* and *centree* sites were averaged by 40% and 60%, respectively, then the overall mean simulated temperature at 26.75 m depth would be -9.55°C, which, ~~It is~~ about 0.75 °C colder than ~~The the~~ temperature recorded in the borehole at the same depth ~~and~~ over the same period of time in the borehole was -8.8°C. Only the modeled soil temperature profile for the *center* site was close to the borehole measurements. If the temperatures from the *rim*, *center*, and *pond* sites were averaged taking into account the proportions of dry tundra (58%), wet tundra (17%), and surface water (25%) following Muster et al. (2012), the overall mean temperature would be -8.7°C.

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Increasing the equilibrium run time for the lake site from 200 years to 400 or 600 years increased the multi-year mean soil temperature at a depth of 26.75 m between 2007 and 2011 from 1.2°C to 0.8 or 0.55°C, respectively.

Similar to those of As with the unfrozen soil thicknesses, the soil temperatures at 26.75 m depth at the lake site were also sensitive to changes in eddy diffusivity and equilibrium run time (Table 6).

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3.3 Effects of (maximum) water depth

For polygon centers with small, when maximum water depths is small, (e.g. 20 and 60 cm), increasing water depth caused a slight increase in the multi-year mean (2003-2011) unfrozen soil thickness (Figure 12a); while for deep polygon centers is deep, e. (e.g. up to 1.2 m), the unfrozen soil thickness started to increase rapidly when the water depth is was about 0.8 m and reached a maximum (of about 8.5 m) at a water depth of around 1.05 m, before it water depth. It decreased again rapidly when for water depths is greater than 1.05 m; increasing either the water depth or the maximum water depth increased the annual mean unfrozen soil thickness (Figure 12). Increasing the water depth in the lake also increased the unfrozen sediment thickness; the sensitivity of the simulated unfrozen sediment thickness was particularly high when the lake water depths of lake were was between 1.0 and 2.0 m (Figure 12b); and very low when the water depth was greater than 2 m. The unfrozen sediment thickness was relatively constant (at about 13 m) when water depth is was greater than 2.0 m. The responses of unfrozen sediment thickness responses were not sensitive to maximum water depths.

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4 Discussion

4.1 Performance of the DOS-TEM

The DOS-TEM can is able to simulate multiple freezing and thawing fronts simultaneously. For example, there was a year-long thawing front on in the sediment yearlong and a freezing and a thawing seasonal front in the water of the lake site; and there were multiple freezing and thawing fronts at the pond site (Figure 10). The simulated thawing fronts and soil/water temperatures at different depths compared very well with analytical Neumann solutions for all three materials, and the accuracy was not sensitive to the depth of bottom-up forcing (Figures 3 and 4). The simulated soil/water temperatures compared reasonably well with in situ measurements from Samoylov Island (Figures 6, 7, 8, and 9).

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Modeling studies usually ~~apply~~ consider thin layers within the ~~top~~ uppermost 1-meter of the soil column to depict daily or seasonal soil temperature dynamics, and then thick layers ~~beneath~~ at greater depths to improve computing efficiency (e.g. Oleson et al., 2004), which may ~~have problem of~~ result in problems when attempting to simulate the thermal dynamics of talik. The ground layering in the DOS-TEM, including snow, water, soil, and bedrock, follows the same strategy. ~~Different~~ Unlike ~~than~~ other models, the DOS-TEM can track multiple fronts, even within ~~one~~ a single layer. The updating of freezing/thawing fronts is based on the Stefan algorithm, which is very efficient. The subsequent updates of temperature ~~of~~ in each layer are similar to those of land surface models using the Crank-Nicolson algorithm, which is also an efficient algorithm. ~~Therefore,~~ The DOS-TEM itself is therefore an efficient model. For example, it ~~only~~ takes only about 10 seconds ~~for the DOS-TEM to~~ simulate a period of 100 years.

~~The simulated thawing fronts and soil/water temperatures at different depths compared very well with analytical Neumann solutions for all three materials, and the accuracy was not sensitive to the depth of bottom up forcing (Figures 3 and 4). The simulated soil/water temperatures compared reasonably well with in situ measurements from Samoylov Island (Figures 6, 7, 8, and 9).~~

~~The simulated thawing fronts and soil/water temperatures at different depths compared very well with analytical Neumann solutions for all three materials, and the accuracy was not sensitive to the depth of bottom up forcing (Figures 3 and 4). The simulated soil/water temperatures compared reasonably well with in situ measurements from Samoylov Island in the Lena Delta, Siberia (Figures 6, 7, 8, and 9). The parameterization used to calculate soil/water temperatures in the DOS-TEM is very efficient. For example, it takes about 10 seconds for the DOS-TEM to simulate a period of 100 years, but it takes more than 30 minutes for a numerical model with apparent heat capacity parameterization to simulate a period of only 10 years on same computer.~~

4.2 Effects of different snowland cover types

The Arctic polygonal tundra contains various a variety of land cover types, e.g. dry polygonal ridges, wet depressed centeres, and water bodies with different of various depths (Boike et al., 2013). These different land cover types all exhibit different exchanges between the land surface and the atmosphere, as well as differences in snow thickness and water depth. In this study, we have mainly investigated the effects of snow thickness and water depth on soil thermal dynamics for the different land cover types. =

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Snow thickness has a strong impact on the soil/water temperatures during cold seasons. At the *rim* site, differences between simulated soil temperatures with and without taking snow drift into account were usually greater than 10°C (Figure 6). At the *center* site, the simulated snow thickness was greater than the measured thickness (Figure 5) and the simulated soil temperatures were warmer than the measured temperatures (Figure 7). The differences at the *pond* site were even greater (Figure 8).

The timing of snowfall is an additional factor affecting the thermal dynamics of soils. The snowfalls simulated for the fall of 2010 were later than the measured snowfalls (Figure 5), which caused early decreases in soil temperatures at the *rim* and *center* sites (Figures 6 and 7). In the real world, early snowfall might be expected to melt in the unfrozen water of the *pond* and *lake* sites; in the modeling, snow accumulated only after the first 2 cm of water was frozen. In the fall of 2010 there was therefore no time-lag between the simulated and measured water temperatures (Figures 8 and 9).

Water ponding has a very important influence on the underlying unfrozen soil thickness (Figure 10) and the permafrost temperature (Figure 11). Our sensitivity tests indicate that, under the present climate on Samoylov Island, the unfrozen soil thickness is very sensitive to water depths of between 1 and 2 m for thermokarst lakes, and between 0.8 and 1.2 m for polygon centers. This has significant implications for the development of talik under thermokarst lakes: following the melting of segregated ice under polygonal tundra (and associated surface subsidence) the development of a thermokarst lake or polygon center can accelerate if the water depth in the lake or pond exceeds a certain threshold. Similarly, talik beneath a thermokarst lake can disappear if the water depth in the lake falls below a certain threshold (van Huissteden et al., 2011).

4.3 Effects of water

Water ponding has a very important influence on the underlying unfrozen soil thickness (Figure 10) and the permafrost temperature (Figure 11). Under the present climate on Samoylov Island our sensitivity tests indicate that the unfrozen soil thickness is very sensitive to water depths of between 1 and 2 m for thermokarst lake; and between 0.68 and 1.2 m for polygonal centre. This has significant implications for the development of talik under thermokarst lakes: following the melting of segregated ice under polygonal tundra and associated surface subsidence the development of a thermokarst lake or polygon centre could accelerate if the water depth in the lake or pond exceeds a certain threshold. Similarly, talik beneath a thermokarst lake could disappear if the water depth in the lake falls below a certain threshold (van Huissteden et al., 2011).

4.3 Limitations and uncertainties

~~Due to~~Because of the harsh Arctic environment, some measurements of atmospheric variables are not available from Samoylov Island and the missing values were replaced with those from the nearby Stolb meteorological station. Air temperatures from the Stolb station (T_{stolb}) compared very well with those from Samoylov Island ($T_{samoylov}$): $T_{stolb} = 0.97T_{samoylov} + 0.65$; $R^2 = 0.99$; $n = 80$. The growing season precipitation at the Stolb station (P_{stolb}) also compared reasonably well with that for Samoylov Island ($P_{stolb} = 0.62P_{samoylov} + 8.35$; $R^2 = 0.53$; $n = 37$), with averages of 26.4 and 29.3 mm/month, respectively. Since there were no precipitation measurements for the cold seasons on Samoylov Island, it is impossible to assess any uncertainty associated with snowfall.

Running ecosystem models for regional or global applications requires large scale reanalysis datasets, such as the global datasets ~~from~~of the Climate Research Unit (CRU), the European Centre for Medium-Range Weather Forecasts (ECMWF), or the National Centers for Environmental Prediction - National Center for Atmospheric Research (NCEP-NCAR). In this study, we compared the air temperature and precipitation from the CRU dataset with those from Samoylov Island. Air temperatures from the CRU were close to those for Samoylov Island in summer, but about 15°C colder in January (Figure 2). The monthly average precipitation in the growing season between 1998 and 2009 was 41.2 mm/month from the CRU and 29.3 mm/month for Samoylov Island. It is clearly important to investigate the uncertainties associated with input data when using models for large scale cold region applications (Clein et al., 2007).

Wind drift is a common process involved in redistributing snow on the heterogeneous landscape of the Arctic tundra (Sturm et al., 2001). There are, however, no measurements of snowfall and snow cover thickness available for the various terrain units of Samoylov Island, making the parameterization of snow drift impossible. Zhang et al. (2012) used snow drift factors and in this study we have set maximal snow thicknesses to simulate the differences in snow thicknesses between different land surface types. However, both methods are very empirical. These measurements will in future need to be collected in situ in order to develop valid parameterizations for snow drift.

The surface temperatures of snow, soil, and water are critical boundary conditions for solving finite difference equations; they are dependent on atmospheric conditions as well as the snow/soil/water conditions (Yi et al., 2013). In models with hourly time steps, snow/soil/water surface temperatures are calculated by iteratively solving the surface energy balance equation for the different surfaces. This involves incoming and reflected solar radiation, incoming and outgoing longwave radiation, sensible and latent heat fluxes between the surface and the atmosphere, and ground heat flux (Oleson et al., 2004). In this study we have used a regression model to calculate surface temperatures on the basis of existing measurements. These algorithms performed better for the *rim* and *center* sites than for the *pond* and *lake* sites.

The exchange of energy in water bodies is not only a result of molecular diffusion and eddy diffusion, but also of other processes such as convection caused by water density instability and complex lake-bottom shapes, which have not been taken into account in this study. We followed Subin et al. (2012) to simulate these effects implicitly by increasing the eddy diffusion coefficient. For example, in order to ~~fit~~agree with the dynamics of water temperatures at bottom of the lake (6 m ~~depth~~) at the *lake* site, the eddy diffusion coefficient had to be increased by at least a factor of 10 (Figure 9). Extensive work is required to test this approach over other lakes in different regions.

~~It is conventional to run models~~Models are commonly run with a multi-year mean climate in order to ~~get~~obtain a state of equilibrium-state, which should ~~be~~only relate ~~to~~the climate and land surface characteristics, and should not be affected by the amount of time used. However, the length of time used for an equilibrium run ~~plays an important role in~~affects the simulated unfrozen soil thickness of polygonal ~~centers~~ and lakes when the water body depth exceeds a threshold value. -For example, it took less than 100 years for the DOS-TEM to reach equilibrium at the *rim* and *center* sites but it ~~did not~~never reached equilibrium at the

lake site, even after 600 years. ~~a on an~~ Therefore, it is vital therefore important to have actual measurements of talik thicknesses beneath water bodies ~~for in order to determine~~ the number of years required for an equilibrium run and ~~for to validate~~ model outputs. Unfortunately, it is not easy to have that information currently. Unfortunately, however, such information is not readily available at present. A new technology known as surface nuclear magnetic resonance, has recently been used over thermokarst lakes to measure the underlying talik thickness (Parsekian et al., 2013), and ~~this method~~ promises to provide useful information on talik that can be used to improve modeling in future studies.

and Lateral heat gradients clearly exist beneath the different land surface types of the polygonal tundra (Figure 11), but since the DOS-TEM is a one-dimensional model it is unable to simulate lateral heat exchange. A 2- or 3-dimensional model would be better able to simulate the thermal processes in complex Arctic tundra landscapes (e.g., Ling and Zhang, 2003; Plug and West, 2009; van Huissteden et al., 2011; Kessler et al., 2012), but such models are difficult to apply over large regions.

Thermal processes vary under the different land surfaces of the heterogeneous polygonal tundra. For example, a talik was present under the lake site, but not under the center or pond sites. In our study we have assumed fixed shapes for polygon centers and ~~for thermokarst lakes, but in future studies~~ it would, however, be desirable to include the dynamics of thermokarst lake development ~~in future studies~~.

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4.4 Outlook

Land surfaces ~~is are~~ heterogeneous at various spatial scales and land surface models (LSMs) with coarse resolutions (usually hundreds of kilometers) ~~use different technologies to take this heterogeneity into account~~ ~~heterogeneity using different technologies~~. Early LSMs only considered the major land surface type within each grid cell (Manabe, 1969); parameters of different land surface types were subsequently aggregated for each grid (Arain et al., 1999). With recent advances in computing power and remote sensing technology, it has become possible to explicitly consider ~~ed~~ different types of land surface, such as those with different plant function types, urban areas, water, etc. (Oleson et al., 2004). Our study has indicated that the heterogeneity of Arctic polygonal tundra results in marked differences in soil thermal dynamics (Figure 10 and 11). In order to simulate methane emissions from polygonal tundra ecosystems on a regional scale it is therefore crucial to distinguish ~~between~~ polygon rims,

polygon centers (with varying water levels), and thermokarst lakes at different stages of development. The sensitivity analysis suggests that it is ~~at least~~ necessary to, at the very least, consider polygon rims, polygon centers (with maximum water depths of less than 0.68 m and with of less than 1.2 m several ~~intervals~~ water depths between 0.68 and 1.2 m), and lakes ~~with water depths of both less than 2 m and greater than 2 m~~. The following steps can be ~~taken~~ used to obtain regional input for the above-mentioned classes:

- 1) The proportion of surface water over regions of polygonal tundra ecosystem can be retrieved from remote sensing albedo datasets (Muster et al., 2013) and the maximal proportion of surface water over different periods ~~calculated~~;
- 2) The distribution of the area covered by polygon centers can be established following Cresto Aleina et al. (2012);
- 3) The relationship between water area and water depth can be established on the basis of in situ measurement data (Wischniewski, 2013).

~~Few measurements of talik thickness beneath thermokarst lakes are available at present. This information is vital for determining the initial conditions and for validating model outputs. For example, it took less than 100 years for the DOS-TEM to reach equilibrium at the rim and center sites but it did not reach equilibrium at the lake site, even after 600 years. A new technology known as surface nuclear magnetic resonance, has recently been used over thermokarst lakes to measure talik thickness (Parsekian et al., 2013). This method promises to provide useful information on talik that can be used to improve modeling in future studies.~~

~~4.5 Limitations and uncertainties~~

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Running ecosystem models for regional or global applications requires large-scale reanalysis datasets, such as the global datasets from the Climate Research Unit (CRU), the European Centre for Medium-Range Weather Forecasts (ECMWF), or the National Center for Environmental Prediction National Center for Atmospheric Research (NCEP-NCAR). In this study, we compared the air temperature and precipitation from the CRU dataset with those from Samoylov Island. Air temperatures from the CRU were close to those for Samoylov Island in summer, but about 15°C colder in January (Figure 2). The monthly average precipitation in the growing season between 1998 and 2009 was 41.2 mm/month from the CRU and 29.3 mm/month for Samoylov Island. It is clearly important to investigate the uncertainties associated with input data when using models for large-scale cold-region applications (Clein et al., 2007).

Wind drift is a common process involved in redistributing snow on the heterogeneous landscape of the Arctic tundra (Sturm et al., 2001). There are, however, no measurements of snowfall and snow-cover thickness available for the various terrain units of Samoylov Island, making the parameterization of snow drift impossible. Zhang et al. (2012) used snow drift factors and in this study we have set maximal snow thicknesses to simulate the differences in snow thicknesses between different land surface types. However, both methods are very empirical. These measurements will in future need to be collected in situ in order to develop valid parameterizations for snow drift.

The surface temperatures of snow, soil, and water are critical boundary conditions for solving finite difference equations; they are dependent on atmospheric conditions as well as the snow/soil/water conditions (Yi et al., 2013). In models with hourly time steps, snow/soil/water surface temperatures are calculated by iteratively solving the surface energy balance equation for the different surfaces. This involves incoming and reflected solar radiation, incoming and outgoing longwave radiation, sensible and latent heat fluxes between the surface and the atmosphere, and ground heat flux (Oleson et al., 2004). In this study we have used a regression model to calculate surface temperatures on the basis of existing measurements. These algorithms performed better for the *rim* and *center* sites than for the *pond* and *lake* sites. The exchange of energy in water bodies is not only a result of molecular diffusion and eddy diffusion, but also of other processes such as convection caused by water density instability and complex lake bottom shapes, which have not been taken into account in this study. We followed Subin et al. (2012) to simulate these effects implicitly by increasing the eddy diffusion coefficient. For example, in order to fit with the dynamics of water temperature at bottom of the lake (6 m) at the *lake* site, the eddy diffusion coefficient

had to be increased by at least a factor of 10 (Figure 9). Extensive work is required to test this approach over other lakes in different regions.

The lateral heat gradients under different land surfaces of the polygonal tundra landscape were obvious (Figure 11). However, the DOS-TEM is a one dimension model, which is therefore unable to simulate lateral heat exchange. A 2- or 3-dimensional model would be better able to simulate thermal processes in complex Arctic tundra landscapes (e.g., Ling and Zhang, 2003; Plug and West, 2009; van Huissteden et al., 2011; Kessler et al., 2012), but such models are difficult to apply over large regions.

Thermal processes vary under the different land surfaces of the heterogeneous polygonal tundra. For example, a talik was present under the lake site, but not under the center or pond sites. In our study we have assumed fixed shapes for polygon centers and for thermokarst lakes. It would, however, be desirable to include the dynamics of thermokarst lake development in future studies.

5 Conclusions

In this study we have modified an ecosystem model to simulate thermal processes under the different land surface types of a polygonal tundra landscape on Samoylov Island, in the Lena Delta of Siberia. The simulated freeze-thaw dynamics and soil/water temperatures compared very well with analytical Neumann solutions for three different materials in idealized runs. Despite a number of limitations and uncertainties relating to model parameterization and data input, the simulated soil/water temperatures compared reasonable well with *in situ* measurements. The modified model is also thus very efficient and is suitable for large-scale regional applications.

Microtopographic relief played has an important role in effect on snow and water cover, which in turn have exert has an important influences on the different thermal processes that operate under the various land surface types. Sensitivity tests have indicated d that thermal processes are very sensitive to changes in water depth when the depth is between approximately 1 and 2 m for lakes, and between 0.68 to and 1.2 m for polygonal center re. The different land surface types of polygonal tundra ecosystems and water dynamics need to be taken into account in large scale ecosystem models, as well as- water dynamics, in order to be able to accurately simulate methane emissions.

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Modeling of thermal processes should at the very least take into account the following land surface types: polygon rims, polygon centers with maximum water depths of less than 1.2 m, and lakes with water depths of both less than 2 m and greater than 2 m.

Appendix A. Updates of fronts and temperatures

The updating of temperatures of snow/water/soil/rock layers consists of two steps: 1) updating of freezing/thawing fronts using the Two-Dimensional Stefan Algorithm (TDSA) method, and 2) updating of temperatures by solving finite difference equations.

The TDSA is based on a well-established Stefan algorithm for determining the positions of freezing/thawing fronts in layered systems (Jumikis, 1977). The TDSA first updates fronts from top-down, and then from bottom-up. In this way, it is able to overcome the problem of overestimating of front positions (Woo et al., 2004). The detailed descriptions of the calculation of the positions of freezing/thawing fronts were presented in Woo et al. (2004), and in Appendix E1 of Yi et al. (2009). Herein we only describe only the changes made to the TDSA.

WhenFor coexisting multiple fronts coexist, previous versions of the TDSA only calculated moving the downward movement of the uppermost front using the surface soil temperature as forcing temperature, and moving the upward movement-up of the lowest front with using the temperature of a specified layer as forcing temperature from bottom. The assumption is that The temperatures between two fronts are assumed to be close to 0°C. This assumption might not be valid for thermokarst lakes, which usually have a year-long thawing front in the sediment-year long (reference). In this study, we implemented top and bottom forcing temperatures for each front. The top-down forcing temperature above forcing is at a specified distance (1 m in this study) above a front are is determined first as shown in Figure A2, which is then used to update the front. Calculations for the below-bottom-up forcing temperatures forcing is are similar to those for above-top-down forcing temperatures. During updating of front position, The energy used for phase changes during the updating of front positions has been recorded for each front.

WhenAfter the freezing/thawing fronts are have been updated, the temperature of each layer is then updated by solving several sets of finite difference equations using the Crank-Nicholson scheme (see Oleson et al., 2004). The number of sets of equations is determined by number of freezing/thawing fronts. If no front exists, then only one set of equations is solved. If one front exists, then two sets of equations are solved, one for the layers above the layer with the front and the part of the layer above the front, and the other for the layers below the layer with front

and the part of the layer below the front. If more than two fronts exist, then three sets of equations are solved: the first set for the layers above the layer with the ~~topmost~~uppermost front and the part of the layer above the ~~topmost~~uppermost front, the second set for the layers below the layer with the lowest front and the part of the layer below the lowest front, and the third equation for the rest of the layers between the ~~topmost~~uppermost and lowest fronts. ~~part between~~The phase change energy determined ~~induring~~ front updating is used as a source term in the equations. ~~Other~~Additional details about information concerning temperature updating can be found in Appendix E2 of Yi et al., (2009).

Appendix ~~AB~~: Modelling the effects of water

The low-centered polygon landscape of the Arctic tundra can be simplified into polygon rims, polygon centers ~~of various sizes~~ (with and without water) ~~of various sizes~~, and lakes of various sizes. On the basis of the original soil and snow structure of the DOS-TEM (the previous version of the DOS-TEM had no water), we modeled water bodies above soil layers (Figure A1a) to simulate the effects that the water in polygon centers and lakes has on freezing or thawing dynamics in the underlying soils or sediments. The division of water into layers was the same as that for soils, i.e. 2 cm, 4 cm, 8 cm, ..., 2^n cm, where n is the layer index.

~~A.1~~ Effects of slope on volumetric water content

The slope between a polygon center and its rim (and also between a lake floor and its shoreline) was set to 28° in our model (Figure ~~A32~~), on the basis of field observations. The vertical distance between the bottom of a polygon center (or of a lake) and the top of its rim was taken to be the maximum water depth (WD_{max}). We assumed the shape of polygon center (or lake) to resemble part of an inverted cone, with a radius of r_{bot} at the bottom and ~~of~~ r_{top} at the top.

The volumetric water content (vwc) of a water layer i can then be expressed as:

$$vwc_i = \frac{V_{top,i} - V_{bot,i}}{V_{cyl}} + \frac{V_{cyl} - (V_{top,i} - V_{bot,i})}{V_{cyl}} \theta$$

where

$$V_{top,i} = \frac{1}{3} \pi r_{top,i}^2 (dx_i + h)$$

$$V_{bot,i} = \frac{1}{3} \pi r_{bot,i}^2 h$$

$$V_{cyl} = \pi r_{top}^2 dx_i$$

$$h = \frac{r_{bot,i}}{\tan(\pi \frac{28}{180})}$$

$$r_{bot} = r_{top} - WD_{max} \tan(\pi \frac{28}{180})$$

In these equations $r_{top,i}$ and $r_{bot,i}$ are the top and bottom radii of layer i , dx_i is the thickness of layer i , h is the vertical distance from the top of the cone to the plane with a radius of $r_{bot,i}$, and θ ($= 0.6$ in this study) is the volumetric water content of the soil rim around the water layers.

Field survey results ~~on~~ the from Samoylov Island indicate that $WD_{max} = 173.1 \ln(r_{top}) - 231.45$ ($R^2 = 0.99$, $n = 12$; Wischniewski, 2013). In Table A1 we present examples for a small polygon, a large polygon, and a lake.

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A.2 Thermal dynamics in water

The exchange of energy within water is affected by several processes including molecular diffusion, wind-driven eddy diffusion, buoyant convection, amongst others. In the DOS-TEM we took into account molecular diffusion, eddy diffusion (which is usually 2-3 orders greater than molecular diffusion; ~~(~~Subin et al., 2012~~)~~), and other processes, by increasing the eddy diffusion coefficient by a factor of between 10 and 100. In cold seasons with snow and ice cover, the dissipation of energy to the atmosphere would only be realized by molecular diffusion, while in warm seasons and with open water the exchange of energy within the water would be much greater. The seasonal variation in energy exchange coefficients is therefore an important factor in the development of unfrozen soil beneath water bodies. Water layers were treated in the same way as soil and snow layers but with different thermal properties (Figure A1a) when calculating the positions of freezing or thawing fronts and the temperatures within water bodies. Following Hostetler and Bartlein (1990), the governing equation for the one-dimensional model is:

$$C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left((G + CK) \frac{\partial T}{\partial z} \right) + \frac{\partial \Phi}{\partial z}$$

where T is the water/soil/snow temperature (K), t is the time (s), z is the depth from water surface (m), C is the volumetric heat capacity (J/(m³K)), λ is the thermal conductivity of water/soil/snow (J/mKs), K is the conductivity due to eddy diffusion (for water only, J/(mKs)), and Φ is a heat source term (w/m²). The detailed parameterization of K and Φ can be found in Hostetler and Bartlein (1990).

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Appendix BC: Soil thermal conductivity

In this study, we applied a soil thermal conductivity scheme proposed by Luo et al., (2009), which integrated the schemes of Johansen (1975) and Côté and Konrad (2005), as follows:

$$k = \begin{cases} K_e k_{sat} + (1 - K_e) k_{dry} & S_r > 1 \times 10^{-5} \\ k_{dry} & S_r \leq 1 \times 10^{-5} \end{cases}$$

$$k_{sat} = \begin{cases} k_s^{1-\theta_{sat}} k_{liq}^{\theta_{sat}} & T \geq T_f \\ k_s^{1-\theta_{sat}} k_{liq}^{\theta_{sat}} k_{ice}^{\theta_{sat}-\theta_{liq}} & T < T_f \end{cases}$$

$$k_s = k_q^q k_o^{1-q}$$

$$k_{dry} = \chi \times 10^{-\eta \theta_{sat}}$$

$$K_e = \frac{\kappa S_r}{1 + (\kappa - 1) S_r}$$

where k , k_{sat} , k_{dry} , k_s , k_{liq} , k_{ice} , k_q , and k_o are thermal conductivities (W/(mK)) of soil, saturated soil, dry soil, soil solid, unfrozen(liquid) water, ice, quartz sand, and other components, respectively. θ_{sat} and θ_{liq} are the porosity and the liquid water content of soil (%), respectively. K_e is the Kersten number. S_r is the soil saturation. χ , η , and κ are 3 parameters whose values for different soil types can be found in Côté and Konrad (2005).

Acknowledgements

This study was supported through grants provided as part of the National Basic Research Program (973 Programme) (2013CBA01807 and 2010CB951402), the Strategic Priority Research Program (XDB030303), and the One Hundred People Plan (O927581001) of the Chinese Academy of Sciences. We are grateful to the German Academic Exchange Service

(DAAD) for providing support for the first author to visit Germany. This work was also supported by the European Union FP7-ENV PAGE21 project (contract number 9 GA282700).

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Table 1. The thermal conductivity, volumetric heat capacity, volumetric water content, and porosity used in idealized runs for water, mineral soils, and organic soils.

	Thermal Conductivity (J/mKs)		Volumetric Capacity (J/m ³)		Heat (10 ⁶ W/m ² K) Volumetric Water Content (%)	Porosity (%)
	Frozen	Unfrozen	Frozen	Unfrozen		
Water	2.29	0.6	2.12	4.19	100	100
Mineral	2.69	1.71	2.06	2.79	33.28	39
Organic	0.37	0.21	0.99	1.84	36.25	90

Table 2. Water and organic soil configurations used in the model for the different test sites.

	Maximum water depth (m)	Water depth (m)	depth	Organic soil
rim	N.A.	N.A.	3 cm	moss (dry organic, porosity (p) = 0.95, volumetric water content (vwc) = 0.3)
			20 cm	organic rich soil (wet organic, p = 0.9, vwc = 0.7)
center	0.25	0	1 m	organic soil (saturated organic, p = 0.9, vwc = 0.9)
pond	1.1	1.05	As for center	
lake	6	6	As for center	

Table 3. Thermal properties of different types of soil on Samoylov Island. The first is derived using soil temperature measurements; the second is calculated using the default scheme in the DOS-TEM.

	Thermal Conductivity (W/mK)		Volumetric Heat Capacity (MJ/m ³ K)		Thermal diffusivity (10 ⁻⁶ m ² /s)	
	Unfrozen	Frozen	Unfrozen	Frozen	Unfrozen	Frozen
Dry organic	0.14/0.17	0.46/0.29	0.9/1.43	0.7/0.75	0.30/0.59	0.66/0.39
Wet organic	0.6/0.30	0.95/0.57	3.4/2.6	1.8/1.44	0.18/0.12	0.53/0.40
Saturated organic	0.72/0.54	1.92/1.83	3.8/4.02	2.0/2.16	0.19/0.13	0.96/0.95
Mineral	N.A./1.00	1.9/2.12	N.A./3.16	2.0/2.04	N.A./0.32	0.95/1.03

Table 4. The root mean squared error ($n = 36,500$) between the thawing fronts (m) from exact Neumann solutions and simulated thawing fronts from the DOS-TEM, with different combinations of total thickness (50, 500, and 5000 m) and bottom-up forcing (b1m: bottom-up forcing at 1 m below front; nobot: no bottom-up forcing) for different materials.

	5000m, b1m	5000m, nobot	500m, b1m	50m, b1m
Water	0.004	1.253	0.032	0.274
Mineral	0.062	4.645	0.177	1.899
Organic	0.012	1.128	0.047	0.065

Table 5. The root mean squared error ($n = 36,500$) between the temperatures ($^{\circ}\text{C}$) from exact Neumann solutions and simulated temperatures from the DOS-TEM for different materials, with 5000 m total thickness and bottom-up forcing at 1 m below the thawing front, at depths of between 0.05 and 20 m.

	0.05	0.1	0.5	1	3	6	9	15	20
Water	0.018	0.017	0.044	0.054	0.039	0.039	0.041	0.087	0.071
Mineral	0.011	0.018	0.014	0.010	0.016	0.027	0.030	0.057	0.062
Organic	0.019	0.016	0.009	0.009	0.024	0.042	0.047	0.111	0.110

Table 6. The simulated multi-year mean (2003-2011) unfrozen soil thicknesses (m)/soil temperature (oC) at 26.75 m depth on at the lake site using different combinations of eddy diffusivities (ke; 1, 10, and 100 indicate the multiplication factor applied to the original value) and equilibrium run time.

	<u>ke1</u>	<u>ke10</u>	<u>ke100</u>
<u>200 yr</u>	<u>8.42/-1.14</u>	<u>9.94/-1.07</u>	<u>10.56/-1.03</u>
<u>400 yr</u>	<u>11.56/-0.67</u>	<u>12.89/-0.61</u>	<u>13.24/-0.59</u>
<u>600 yr</u>	<u>13.71/-0.40</u>	<u>15.72/-0.34</u>	<u>16.11/-0.32</u>

Table A1. The area, top radius (r_{top}), bottom radius (r_{bot}), maximum water depth (WD_{max}) of polygons or lakes, and their volumetric water contents (vwc) at the top and bottom.

	Area (m^2)	r_{top} (m)	r_{bot} (m)	WD_{max} (m)	VWC	
					Top layer	Bottom layer
Small polygon	50 [*]	3.99	3.95	0.08	1	0.99
Large polygon	200 [§]	7.98	7.30	1.28	1	0.94
Lake	39541 ^{&}	112.19	109.07	5.86	1	0.98

* Mean average surface area of the smallest polygon centers on Samoylov Island (Wischnewski, 2013);

[§] Mean average surface area of the largest polygon centers surveyed on Samoylov Island;

[&] Area of the large thermokarst lake on Samoylov Island.

Figure 1. (a) Circumpolar permafrost distribution (Brown et al., 1998) and the Lena River Delta; (b) Location of the Samoylov study site within the Lena River Delta, Eastern Siberia (NASA, 2000); and (c) ~~locations of the measurement~~ locations ~~on the~~ Samoylov Island.

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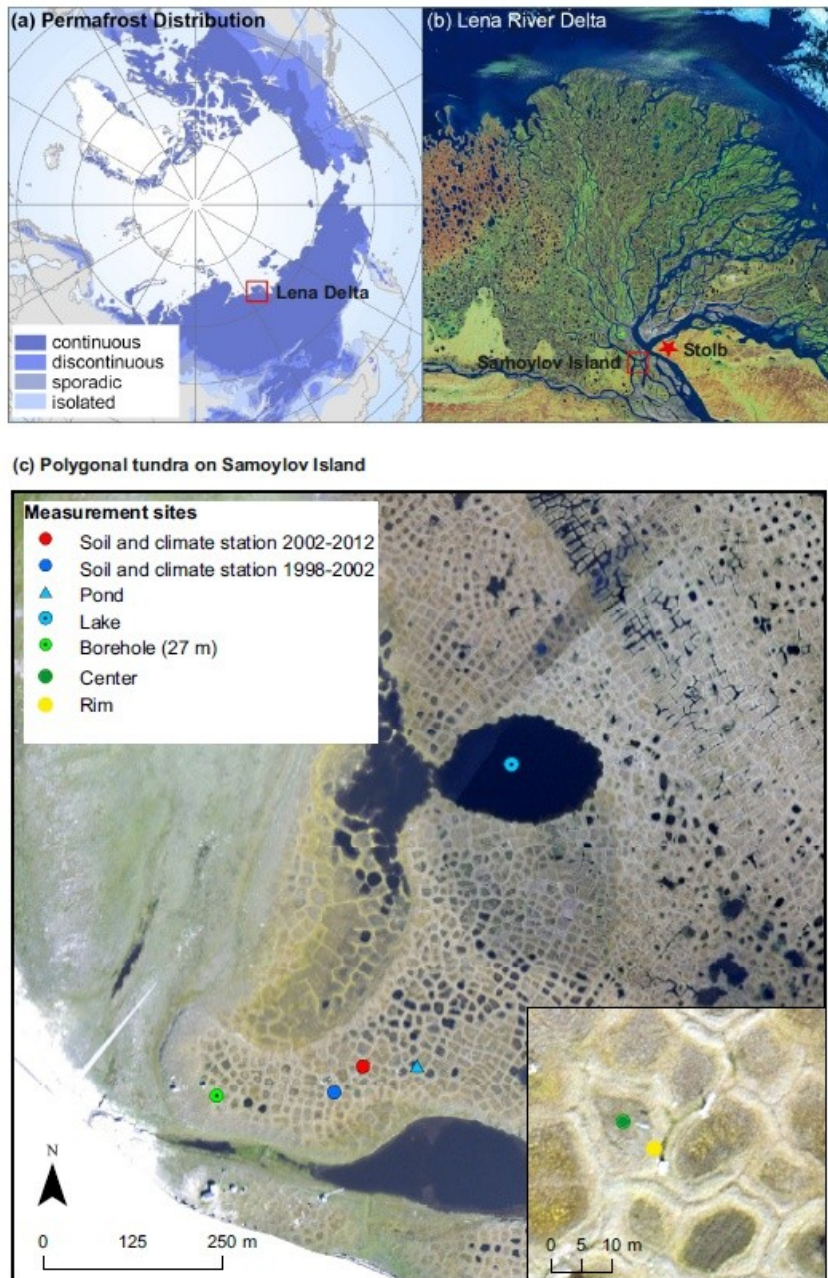


Figure 2. Monthly air temperature (Ta) and precipitation (P) measurements from Samoylov Island (Samoylov), Stolb meteorological station (Stolb), and from the Climate Research Unit global dataset (CRU)

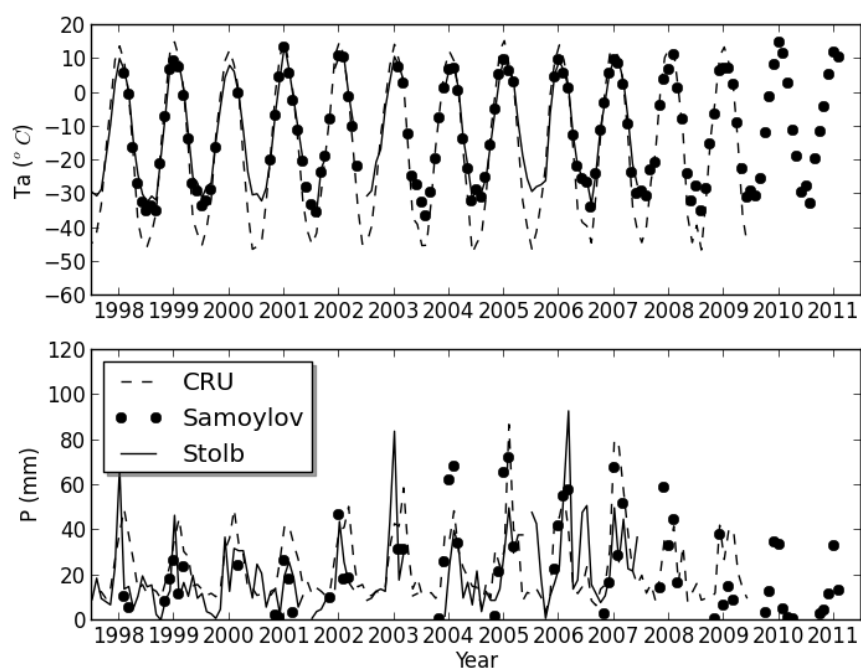


Figure 3. Comparisons of outputs from DOS-TEM simulations, exact Neumann solutions (Exact), and Stefan's equation (Stefan) for [1a](#)) water, [2b](#)) mineral soil, and [3c](#)) organic soil over a one hundred year period. The term B50CM means simulations from the DOS-TEM with bottom-up forcing at 50 cm beneath the lowest freezing or thawing front, and likewise for other similar terms. NOBOT means no bottom-up forcing. The outputs from the DOS-TEM have been plotted for the middle of every tenth years and different cases have been started from different years in order to make the figures more readable.

[2](#)

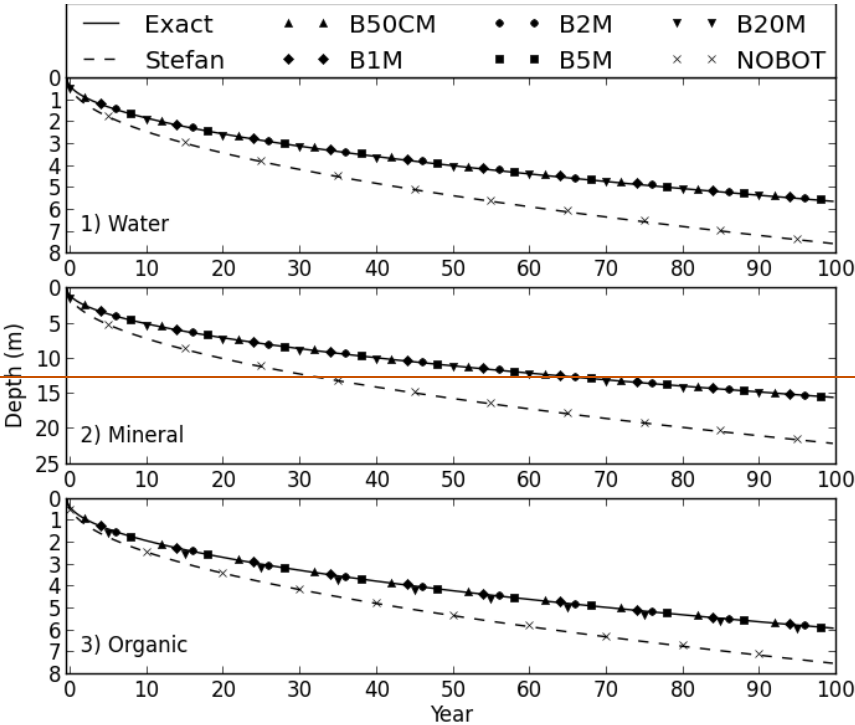
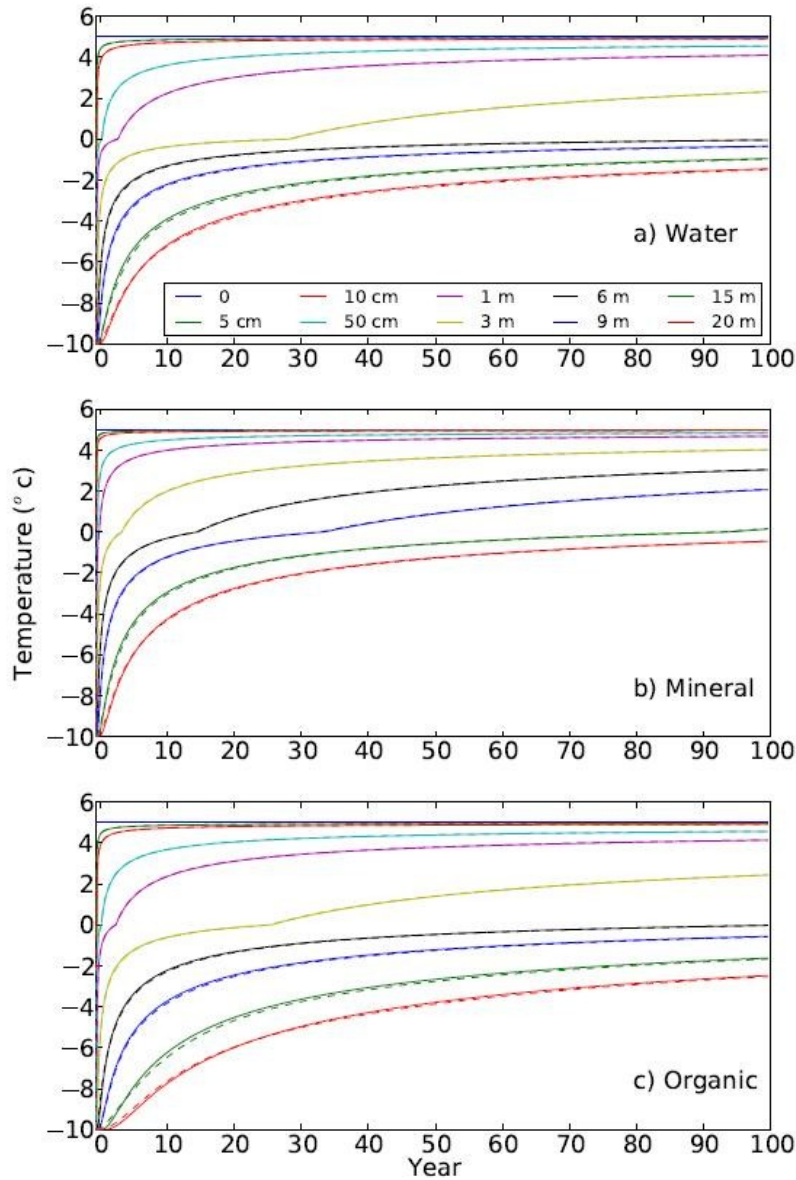


Figure 4. Comparisons of outputs from DOS-TEM simulations (dashed lines) and exact Neumann solutions (solid lines) for **1a)** water, **2b)** mineral soil, and **3c)** organic soil over a period of one hundred years, at depths from 0 cm to 20 m.



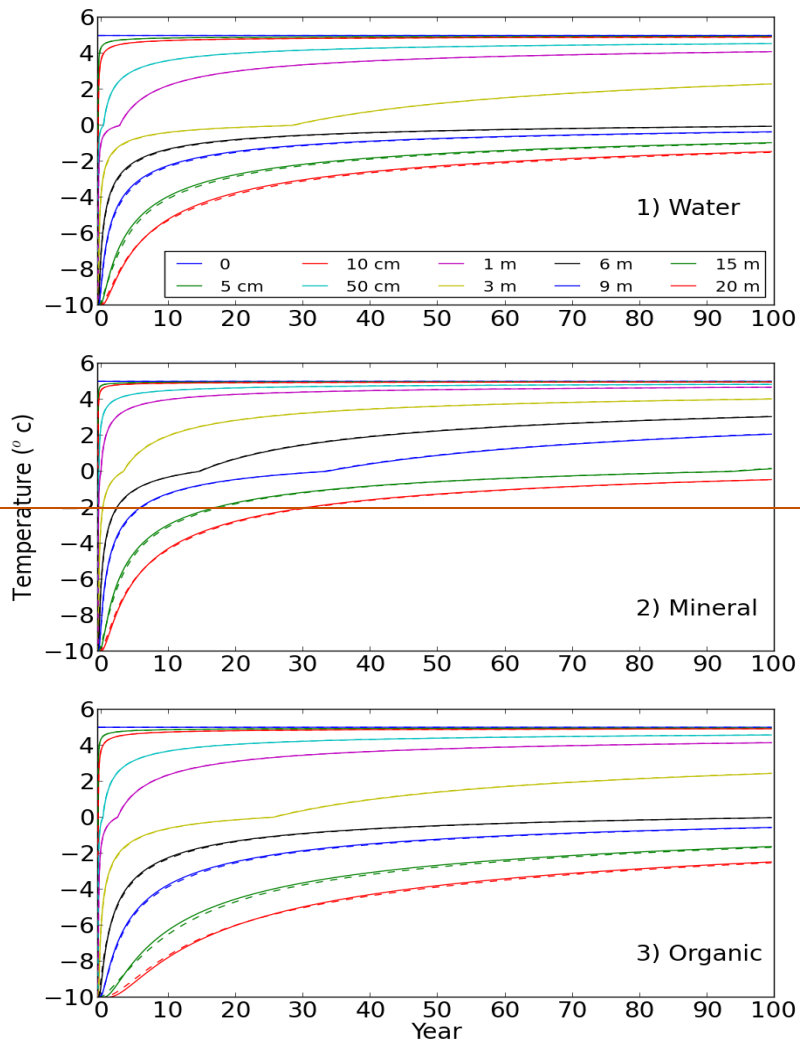
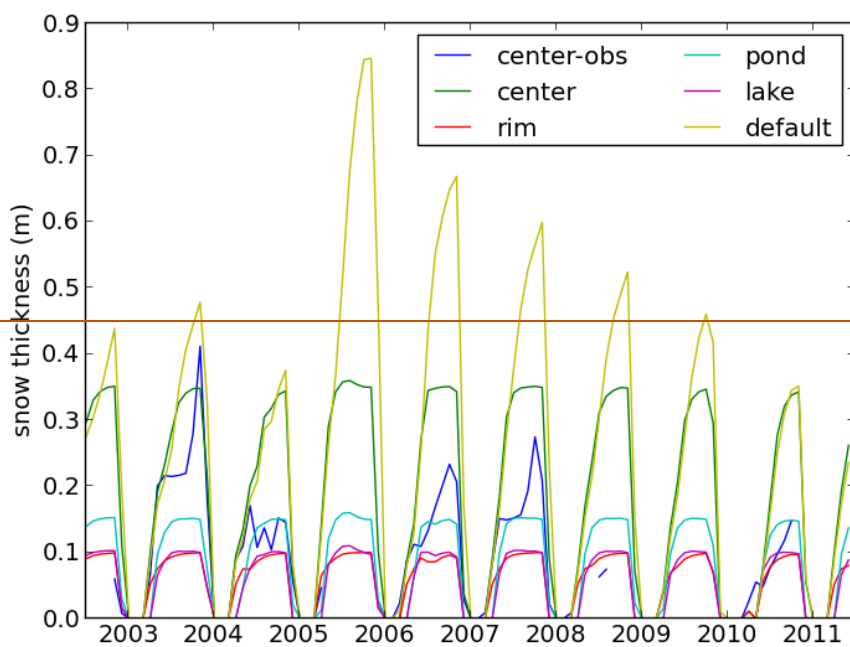
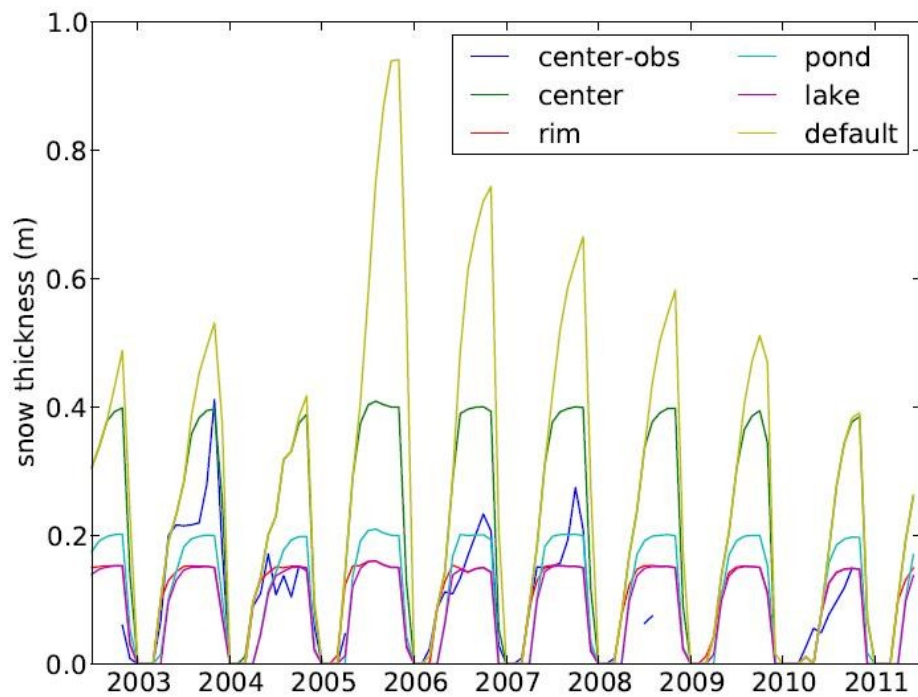


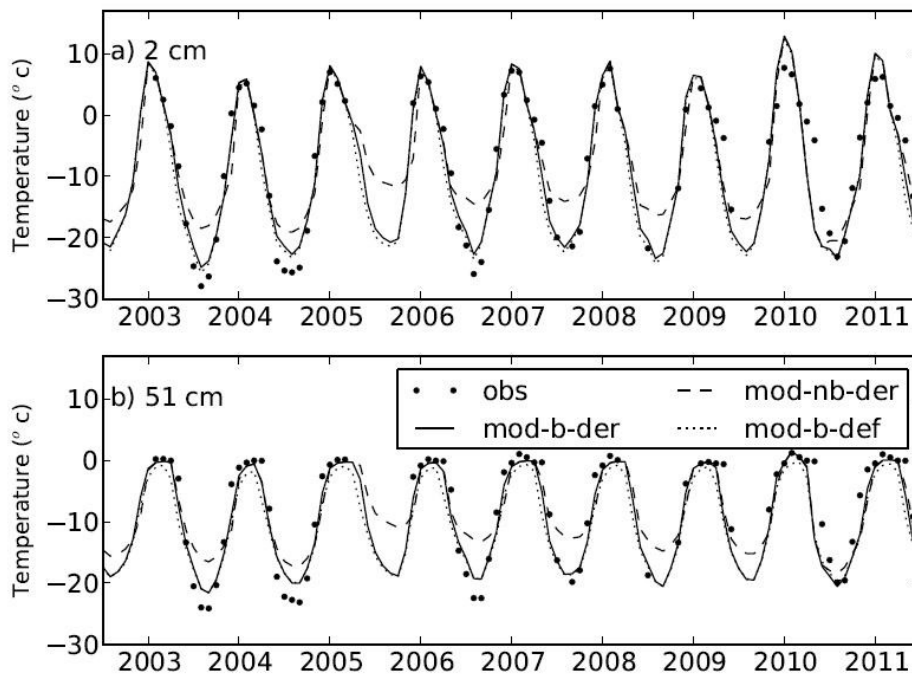
Figure 5. Comparisons of simulated maximum (monthly) snow thicknesses at the *center*, *rim*, *pond*, and *lake* sites, the default values (with no maximum snow thickness set), with those from field measurements at the *center* site (center-obs), over the period from 2003 to 2011.

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Figure 6. Comparisons of monthly average soil temperatures at 2 cm and 51 cm depth below the *rim* site from simulations (mod), with and without a maximum snow thickness (b and nb), using derived and default thermal properties (der and def), with those from field measurements (obs), over the period from 2003 to 2011.



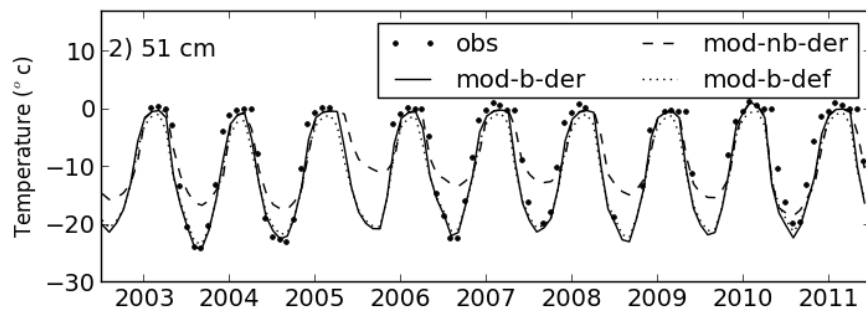
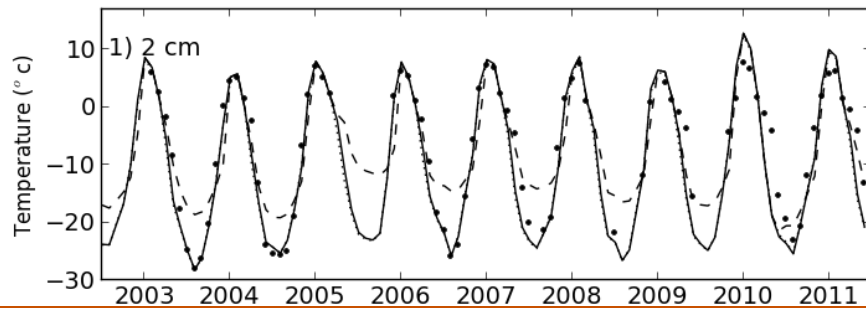
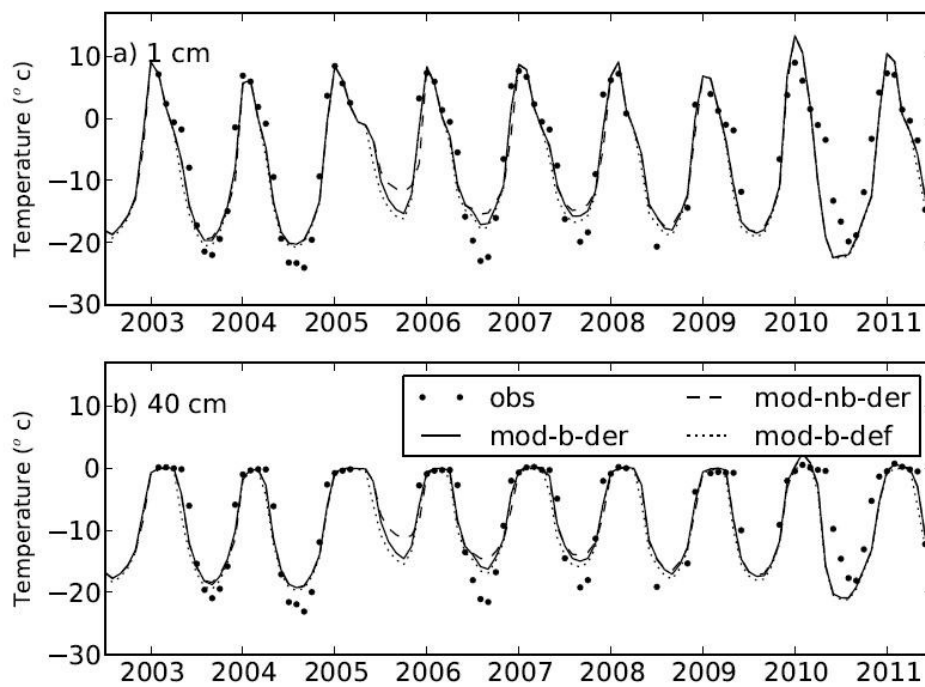


Figure 7. Comparisons of monthly average soil temperatures at 1 and 40 cm depth below the *center* site from simulations (mod) with and without a maximum snow thickness setting (b and nb), using derived and default thermal properties (der and def), with those from field measurements (obs), over the period from 2003 to 2011.



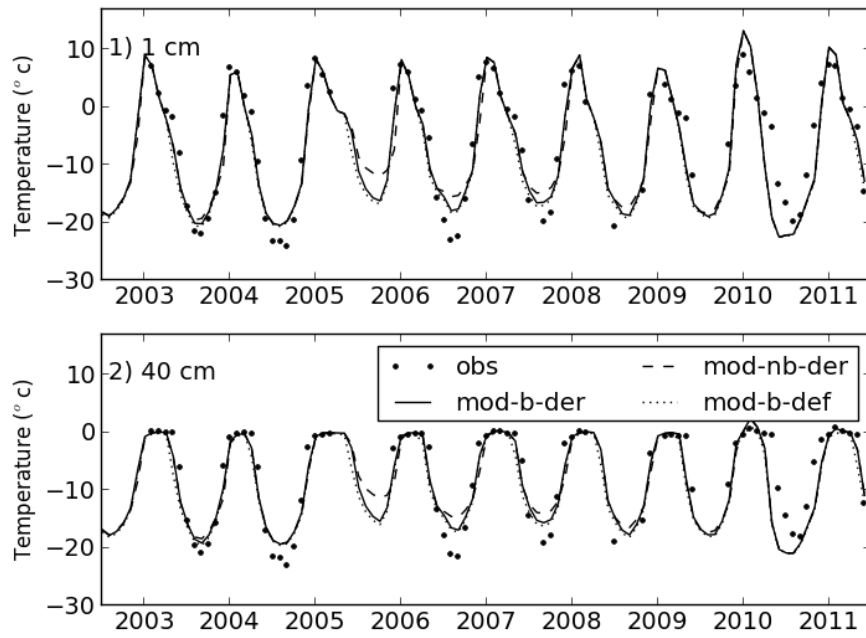
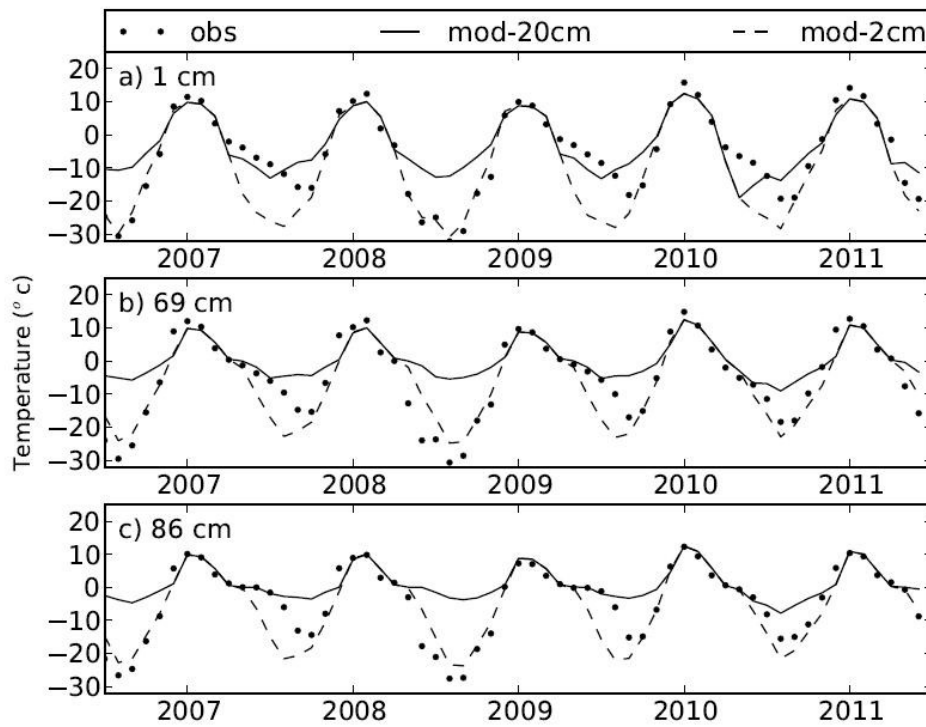


Figure 8. Comparisons of monthly average water temperatures at 1, 69 and 86 cm depth below the water surface at the *pond* site from simulations with 15 cm (mod-15cm) and 2 cm (mod-2cm) maximum snow thickness, over the period from 2007 to 2011.

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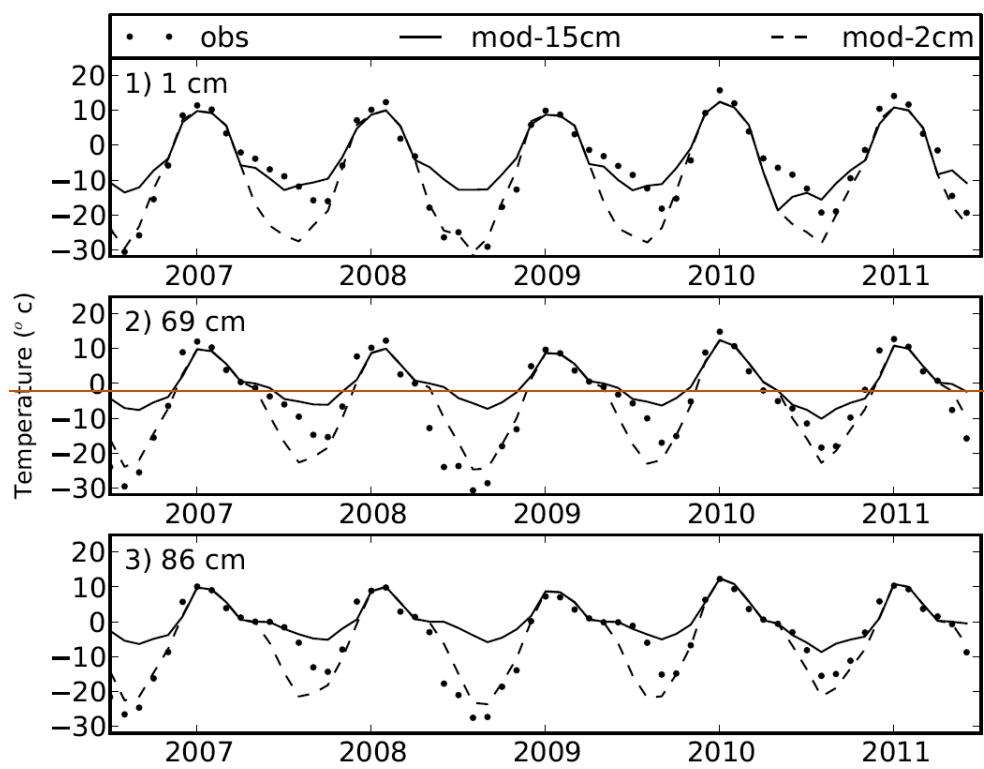
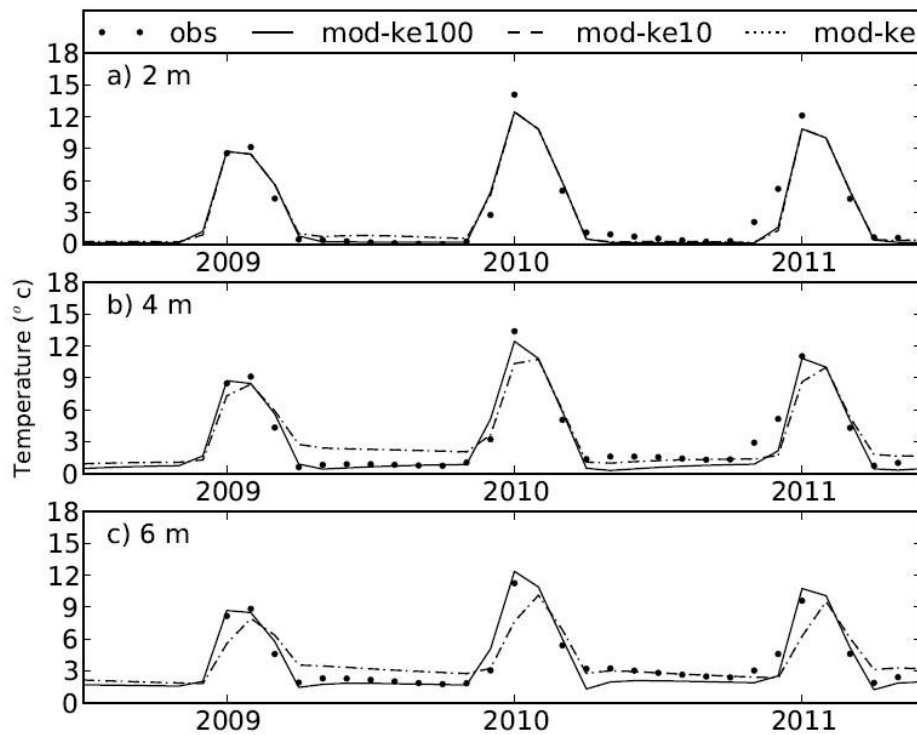


Figure 9. Comparisons of monthly average water temperatures at 2, 4 and 6 m below the water surface at the *lake* site from simulations (mod) using default, 10 times, and 100 times the eddy diffusion coefficient (ke, ke10, and ke100) with field measurements (obs) over the period from 2009 to 2011.



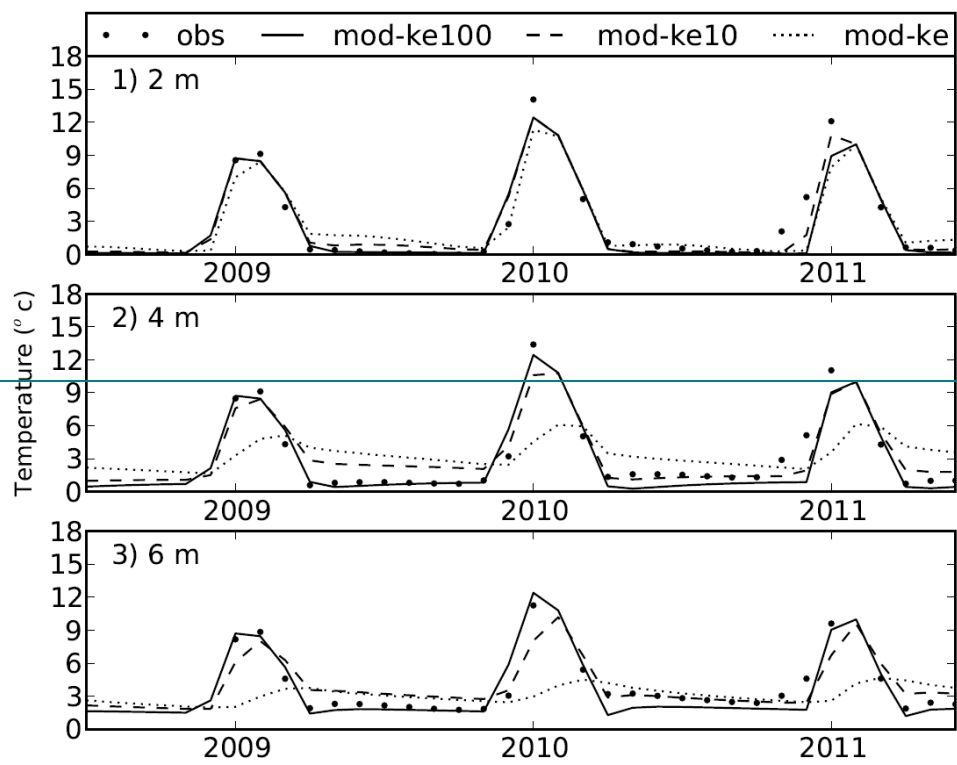
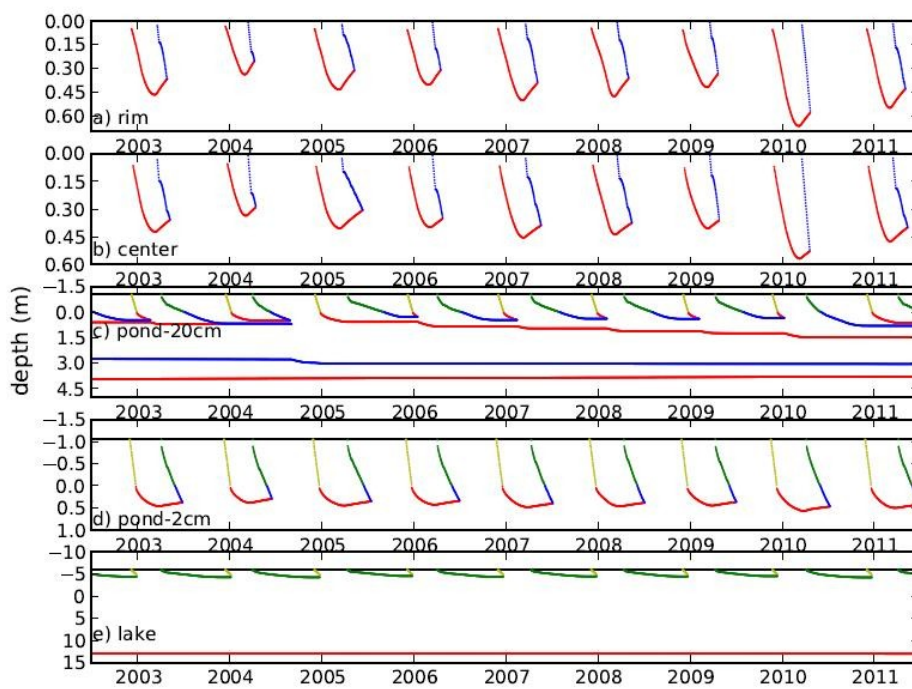


Figure 10. Simulated soil freezing (blue) and thawing (red) fronts, and water freezing (green) and thawing (yellow) fronts (depths in meters) over the period from 2003 to 2011 for **1a**) the rim site, **2b**) the center site, **3c**) the pond site with 15 cm maximum snow thickness, **4d**) the pond site with 2 cm maximum snow thickness, and **5e**) the lake site. The surface of the soil was taken to be at 0 m depth, with the downward direction positive and the upward direction negative.



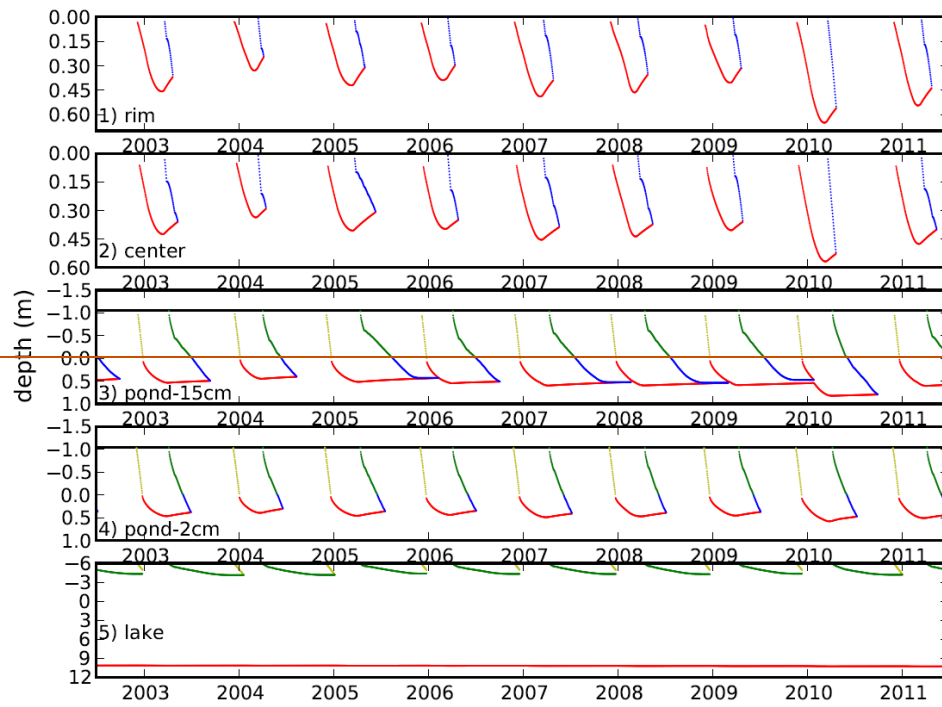
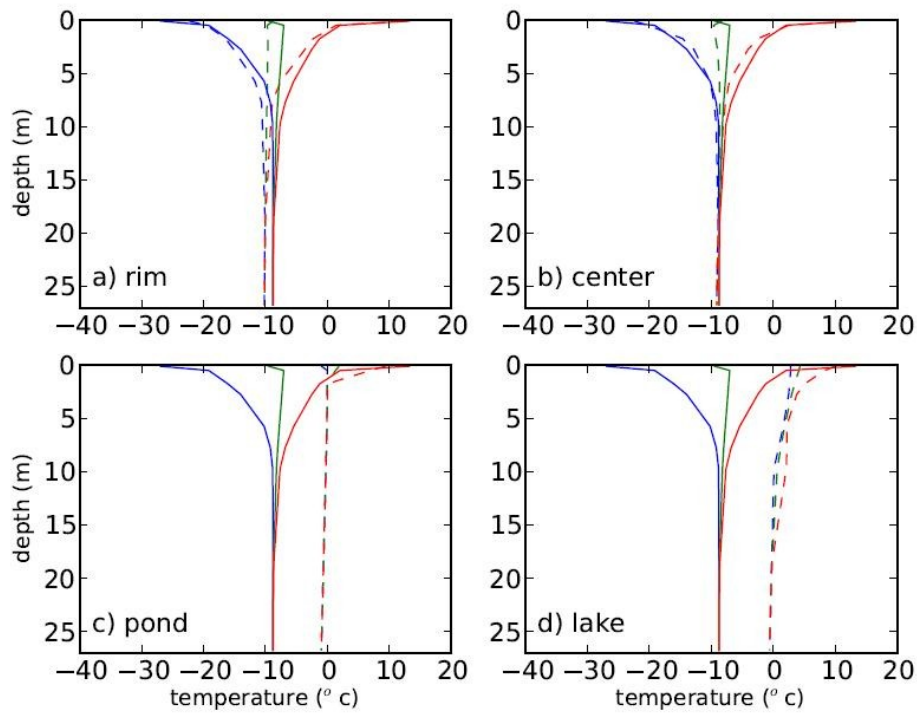


Figure 11. Comparisons between simulated (dashed lines) and measured (solid lines) values for annual mean (green), maximum (red), and minimum (blue) soil temperatures ($^{\circ}\text{C}$) averaged over the period from 2007 to 2011 for the **1a**) rim, **2b**) center, **3c**) pond, and **4d**) lake sites



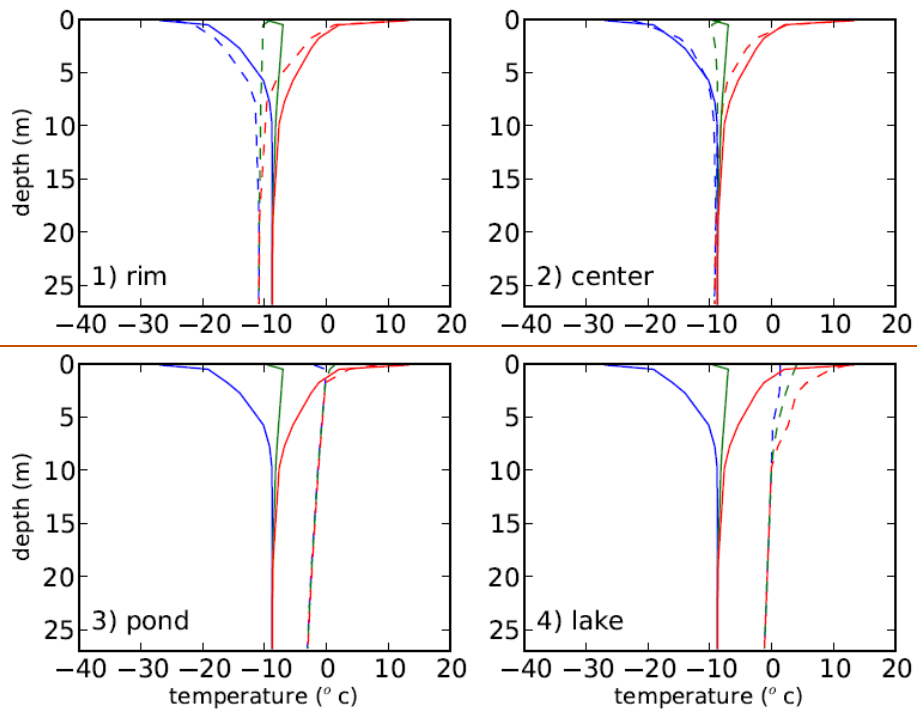
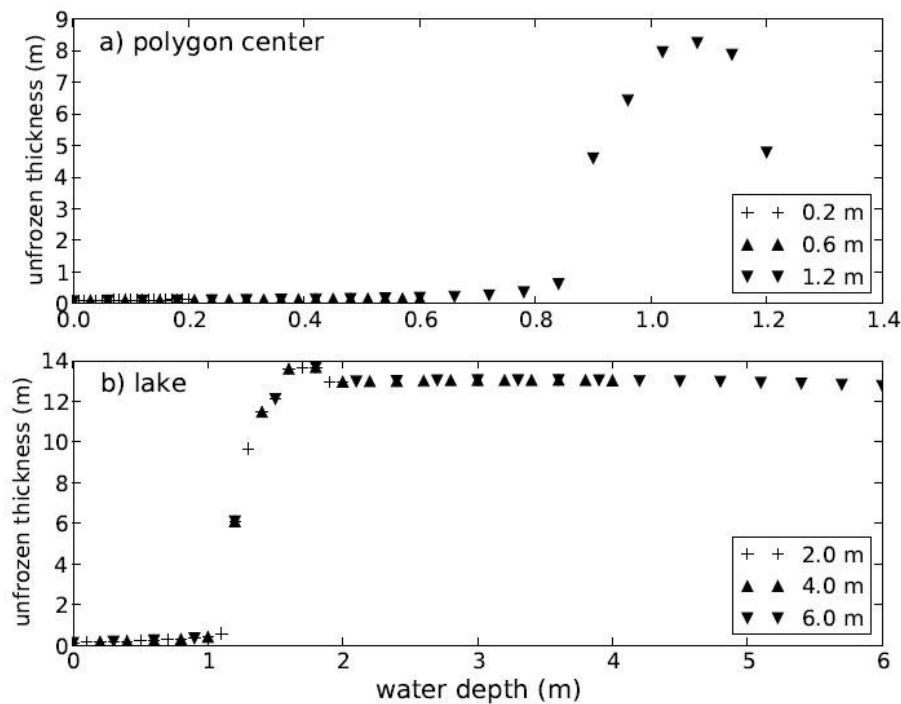


Figure 12. Effect that water depth in polygon centers/lakes has on the mean unfrozen soil thickness over the period from 1981 to 2011. For polygon centers depths in a), shallow = 20 cm, medium = 60 cm, and deep = 120 cm. For lake depths in b), shallow = 2 m, medium = 4 m, and deep = 6 m. Empty, half full, and full refer to water depths that are 0%, 50%, and 100% of the maximum polygon center/lake depth, respectively. Responses of simulated multi-year mean (2003-2011) unfrozen soil thickness, to changes ~~of~~in water depths in a) polygon centers (with maximum water depths of 0.2, 0.6 and 1.2 m) and b) lakes (with maximum water depths of 2.0, 4.0 and 6.0 m).



批注 [E12]: The layout of this caption seems a little strange and may require some attention!

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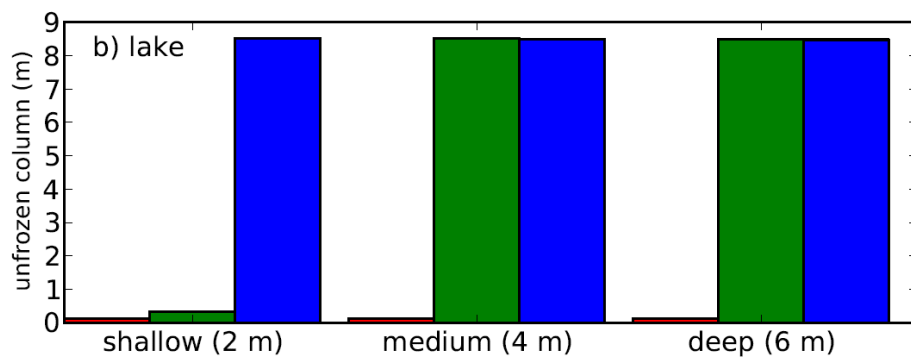
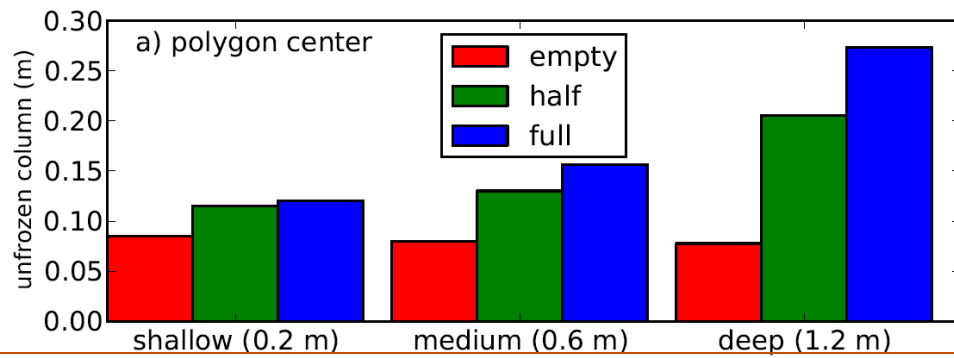
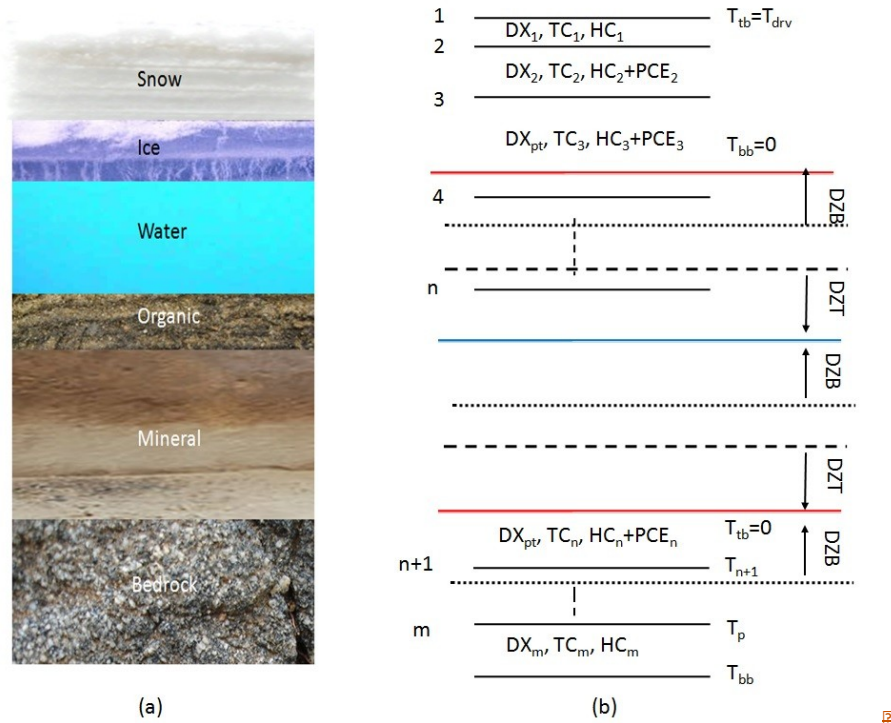
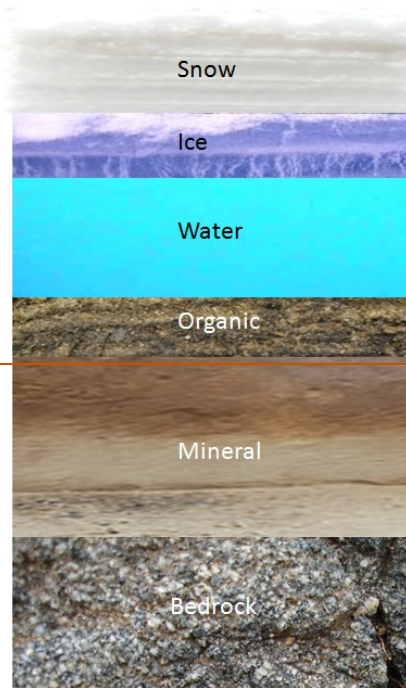
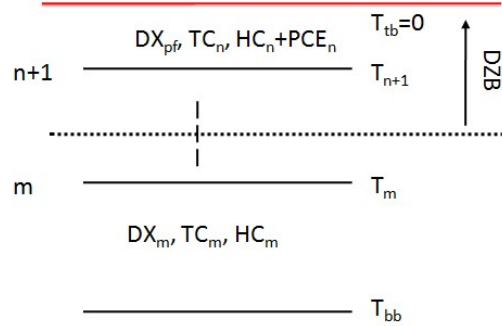
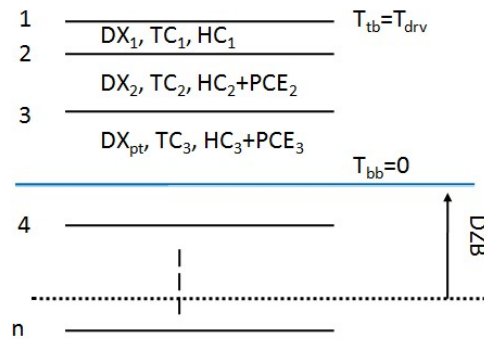


Figure A1. The ground components considered in the DOS-TEM (a), and a diagram of updating freezing and thawing fronts of ground components, together with temperatures (b). DX, TC, HC, and PCE stand for thickness, thermal conductivity, heat capacity, and energy used for phase change, respectively; there are altogether m layers, n and m are layer indexes; DZT and DZB are the distances between the top-down and bottom-up driving depths (dashed and dotted horizontal lines) and the depth-position of the front. Freezing and thawing fronts are indicated with blue and red solid lines, respectively. Vertical dashed lines indicate layers not shown. T_{tb} , T_{bb} , and T_{drv} are the top boundary, bottom boundary and ground surface driving temperatures, respectively. The T_{bb} at the bottom of the ground structure is determined by the temperature and thermal properties of the overlying layer and the prescribed heat flux.



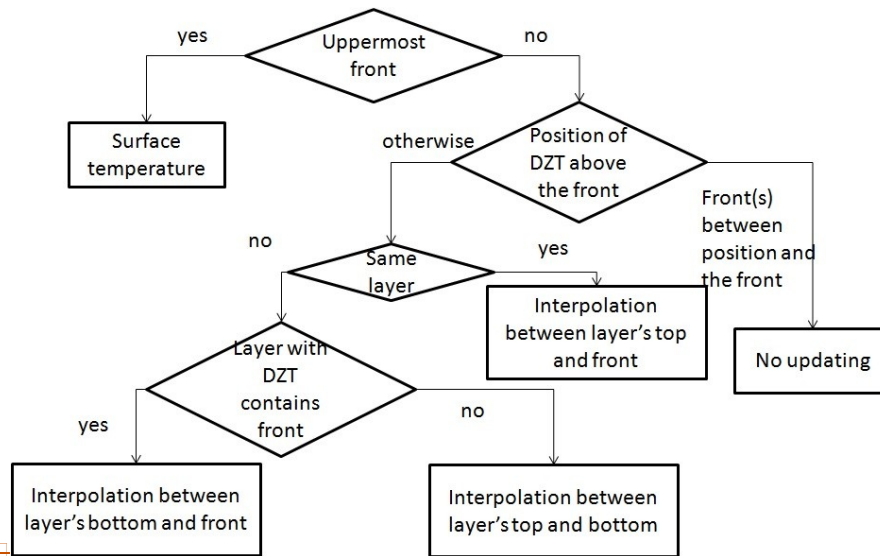


(a)



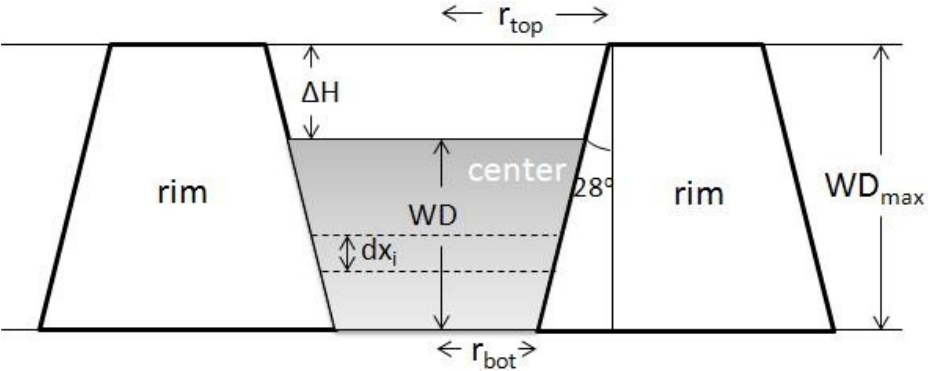
(b)

Figure A2. The flowchart ~~for the determining calculation~~ of upper temperatures for updating the position of the front from ~~upside~~ above. (note: Front(s) between position and the front in the flow chat means there are front(s) between the front under consideration and the position of forcing (DZT above the front)).



批注 [E13]: In the figure, I don't know what you mean by "Front(s) between position and the front". (What position?)

Figure A2A3. Diagram of polygon rim and polygon centerpond/lake, in which r_{top} is the radius of the top and r_{bot} that of the bottom of a polygon centerpond or lake; WD and WD_{max} and ΔH are the water depth, and maximum water depth, and the microtopographic relief height in a polygon centerpond or lake, respectively.



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