Journal of Hydrology: Regional Studies 39 (2022) 100975

Contents lists available at ScienceDirect

Journal of Hydrology: Regional Studies

journal homepage: www.elsevier.com/locate/ejrh

Integrated surface-subsurface water and solute modeling of a reclaimed in-pit oil sands mine: Effects of ground freezing and thawing

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ARTICLE INFO

Keywords:
Oil sands
Mine reclamation
HydroGeoSphere
Surface water – groundwater interactions
Ground freeze-thaw

ABSTRACT

Study region: Athabasca Oil Sands, Alberta, Canada.
Study focus: The upland and wetlands substrate in reclaimed oil sands landforms will be constructed of post-mining materials with an objective of replicating the landscape and hydrology of the surrounding boreal systems. Porewater in these materials contain elevated levels of salts and other solutes. Water quality will govern the success and sustainability of the reclaimed landscape. Tightly coupled water and heat dynamics control water and solute movement in boreal systems. We used three-dimensional integrated surface-subsurface flow and chloride transport models with and without ground freezing-thawing to compare performance of an in-pit oil sands mine currently being reclaimed.
New hydrological insights for the region: Transient simulations under wet/dry climate cycles suggest that the reclaimed landform will shed water only during wet years. Annual water balance with and without coupled heat dynamics is identical. However, the three-dimensional representation of ground freeze-thaw results in reduced snowmelt infiltration, summer groundwater table, and solute release during winter. The outcome is increased spring runoff, 20% decrease in chloride mass release over simulated eight-year wet climate cycle and relatively reduced summer runoff. The model results suggest that (1) coupled heat dynamics should be considered for detailed evaluation of reclaimed in-pit landforms at finer time scales, and (2) modeling reclaimed landforms without freeze-thaw provides conservative annual solute release estimates, which is appropriate for coarse site-wide models.

1. Introduction

The Alberta oil sands are located in the Canadian boreal plains. The oil sands mines reaching end of operations are being progressively reclaimed. As per regulations, oil sands mines are to be reclaimed to a land capability that is equivalent to pre-mining conditions (i.e., locally common boreal ecosystems) (AER 2018). Specifically, the reclaimed landforms are expected to provide an equivalent capability to store and transmit water while merging into the surrounding boreal landscape (Ketcheson et al., 2017; Nagare et al., 2018; Biagi et al., 2021). Water quality and water budget within reclaimed oil sands landscapes need to be evaluated to predict

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https://doi.org/10.1016/j.ejrh.2021.100975
Received 7 July 2021; Received in revised form 31 October 2021; Accepted 5 December 2021
Available online 9 December 2021

the sustainability of the closure drainage designs and to demonstrate alignment with proposed end land-use objectives (Ketcheson et al., 2016; Biagi et al., 2019, 2021; Hartsock et al., 2021). Water movement in boreal regions is characterized by tight surface water and groundwater coupling wherein evapotranspiration makes up the majority of outflow (Hayashi et al., 1998a; Laudon et al., 2007; Devito et al., 2012; Smerdon et al., 2007; Ketcheson et al., 2017). Given the cold regions climate of oil sands region, water and solute cycling is driven by both water and heat dynamics (Hayashi et al., 1998a, 1998b; Devito et al., 2012; Ketcheson and Price, 2016a; Huang et al., 2018; Biagi and Carey, 2020). Oil sands mine reclamation designs need to incorporate these hydrological characteristics of the boreal regions.

Oil sands mines are being reclaimed using mined out materials (e.g., peat, overburden, tailings sand) that is stockpiled during mining. Use of these materials presents water quality challenges for revegetation and water discharge from reclaimed landscape. For example, tailings sand is used to construct in-pit tailings landforms and the hydraulically placed sand holds oil sands process affected water (OSPW) which contains elevated levels of salts and other constituents of interest (COIs). Understanding mobility of these COIs by meteoric water during wet climate cycles and water availability for vegetation and end pit lakes during dry climate cycles is essential for the proper evaluation of reclamation designs (Kessler et al., 2010; Ketcheson et al., 2016; Nagare et al., 2018). Water recharging on uplands flushes the shallow subsurface materials and discharges salts and COIs to low-lying areas in reclaimed landscapes, a process that mimics the functioning of natural boreal upland - wetland systems (Smerdon et al., 2005, 2007; Kessel et al., 2018; Nagare et al., 2018). Such flushing and upward movement of water in unsaturated zone by capillary action can evapoaccumulate salts and COIs in root zone and on surface of the wetlands and uplands (Dobchuk et al., 2012; Rezanezhad et al., 2012; Ketcheson et al., 2016; Simhayov et al., 2017; Nagare et al., 2018). Therefore, performance evaluations of reclamation designs compare nature of surface water and groundwater interactions, location of groundwater table, solute flushing mechanisms and water volume and solute mass release rates from the landforms to design criteria and feed the results into the engineering process for design optimization. Solute cycling within the landform includes advective flushing of the hummocks and diffusive flushing of the underlying fine tailings (Dobchuk et al., 2012; Nagare et al., 2015a, 2018; Biagi et al., 2019). The groundwater table location governs geotechnical and hydrotechnical stability of the landform (Nagare et al., 2018). It also governs the salinization potential of the root zone of the treed upland vegetation (Dobchuk et al., 2012; Nagare et al., 2015a, 2018). Understanding of surface water groundwater interactions, flushing of shallow subsurface and salinization potential of the root zone is the main driver for cover soil design research in oil sands reclamation. This includes investigations of changes in properties of covers due to freeze-thaw, thickness requirements to offset salinization by upward movement of water and changing role of cover soils in hydrology of reclaimed slopes with aging (Kelln et al., 2008; Kessler et al., 2010; Meiers et al., 2011; Ketcheson and Price, 2016b).

Numerical models are often used to analyze water and solute cycling within design landscapes (Dobchuk et al., 2012; Huang et al., 2018; Lukenbach et al., 2019; Nagare et al., 2018). There is no consistency of models used to represent constructed systems in the oil sands region, as models have been chosen and developed to examine a specific process or operational questions, focusing on decoupled overland/groundwater flow or inorganic solute transport (Biagi and Carey, 2020). Furthermore, these models are often too simplistic, often one- or two dimensional and do not comprehensively represent all the hydrological processes (e.g., evapotranspiration, frozen ground, etc.) that govern the water and solute cycling in reclaimed landforms (Biagi and Carey, 2020; Nagare et al., 2015a, 2018). Frozen ground in reclaimed landforms can impede infiltration and increase overland flow during spring melt (Ketcheson and Price, 2016a), ground frost in wetland can delay groundwater outflow (Ketcheson et al., 2017) and snowmelt rate and partitioning can govern the timing of combined runoff from a reclaimed oil sands landform (Biagi and Carey, 2020). These processes can lead to increased freshwater outflow from reclaimed landforms, a process critical to sustainability (water quality and quantity) of downstream end pit lakes. Despite of its critical importance, ground-freeze thaw is rarely incorporated in analysis of hydrology of reclaimed oil sands landforms (Biagi and Carey, 2020). Given the tightly coupled surface water and groundwater processes in boreal settings, integrated surface water and groundwater flow and solute transport modeling is well suited to evaluate post-closure landscape performance (Smerdon et al., 2005, 2007; Price et al., 2010; Carrera-Hernández et al., 2011; Nagare et al., 2015a, 2018). There are not many examples of integrated modeling, let alone with ground-freeze thaw, to support oil sands mine reclamation designs. Integrated models have the capability to simulate coupled water and heat dynamics (Schilling et al., 2019) but such simulations may come at an increased computational cost and effort to parameterize the model (Huang et al., 2018). It is therefore important to strike a balance in inclusion of details of processes while using integrated models to support evaluation of reclaimed landforms.

In this study, we demonstrate the combined use of a three-dimensional (3D) integrated flow and solute transport model and a one-dimensional (1D) coupled flow and heat transport model to analyze water and solute dynamics with frozen ground processes in an in-pit oil sands mine currently under reclamation. The reclaimed mine consists of coarse sand tailings hummocks draining into low-lying flatter areas, similar to the general boreal setting of treed uplands surrounded by organic wetlands. The objective of the study was to develop a practical coupled water, heat and chloride transport modeling approach using physically based integrated models to support oil sands mine reclamation. The 3D modeling included the most important hydrological and solute transport processes (e.g., surface-atmosphere interactions, snowmelt rate and timing, frozen-ground processes, unsaturated zone processes, and overland/subsurface flow and transport). Coupling the 1D and 3D models ensured striking a reasonable balance between inclusion of details of processes, and computational burden and parameterization effort. Specifically, we investigated the effect of frozen ground on spring melt runoff rate, timing and outflow water quality, changes to seasonal groundwater table location, and annual water and solute balances when frozen ground processes are included and excluded from the model. There is limited direct data from the reclaimed landform to confirm the model performance. Data from other compatible reclaimed and natural sites was used to validate the model performance. The modeling results are being used as a guide to optimize reclamation processes and to develop monitoring plans once the landform is fully reclaimed.

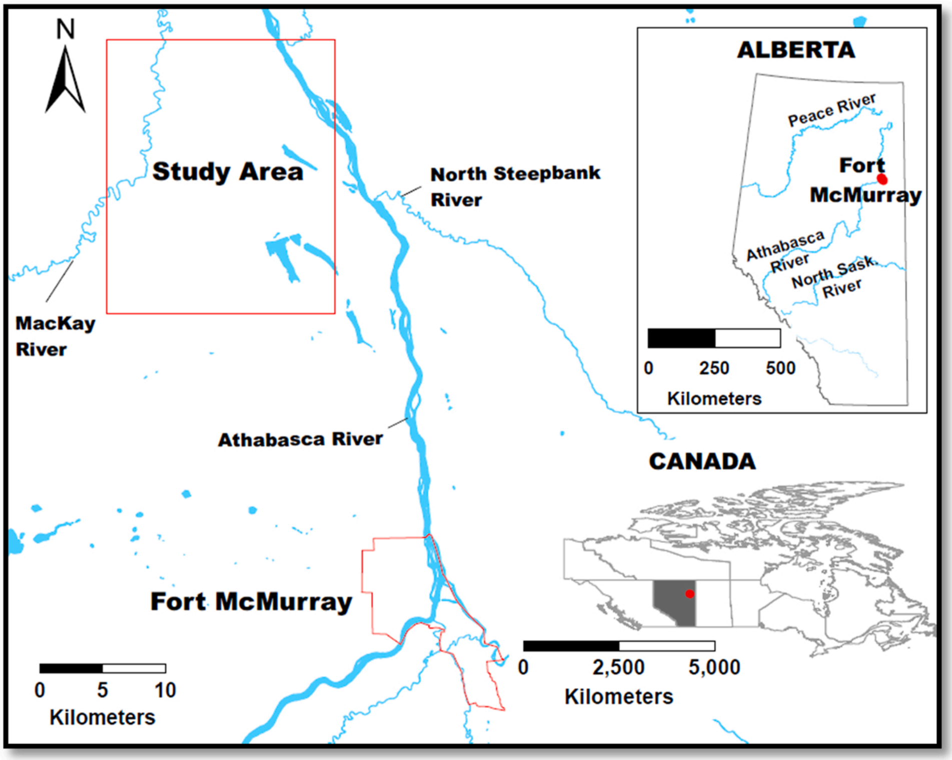

Fig. 1. Location map.

2. Methods

2.1. Study case example

The reclaimed mine pit site is an in-pit mine currently being reclaimed by Syncrude Canada Ltd. (Syncrude). Syncrude mine site is located 40 km north of Fort McMurray, Alberta, Canada. The study area is shown in Fig. 1. The area of the reclaimed watershed modeled in this study is 8.4 km^2. The reclamation design was completed over multiple years in the past decade. The mine pit was backfilled with a mixture of fluid fine tailings and sand tailings (together called composite tailings or CT). To create upland/wetland systems typical of coarse textured natural systems in the boreal forests, the CT filled pit is being covered with a series of upland sand hummocks (Fig. 2). The area between hummocks form swales/valleys and the hummock/swale system is sloped towards a flat low-lying area connected to the landform outlet. At closure, the outlet of the reclaimed landform will be connected to an end pit lake by a surface closure channel. The hummocks and the low-lying area are being covered with soil covers to promote vegetation growth. At reclamation, the elevated sand tailings hummocks will support treed vegetation and drain into the low-lying wetland areas. The low-lying area is intended to evolve into a wetland supporting native wetland vegetation species. The soil covers comprise of an upper layer of salvaged peat overlying a layer of salvaged glacial clay soil (Dobchuk et al., 2012; Nagare et al., 2018). As already introduced, the tailings (sands and CT) are constructed primarily by hydraulically transporting in OSPW and therefore contain elevated levels of saline pore-fluid at their placement.

The model layers (bottom to top) consist of thick composite tailings that filled the pit at end of mining. The CT is covered by a minimum 1 m thick tailings sand cover throughout the model domain. The tailings sand cover is overlain by tailings sand hummocks (1 – 10 m thick) in areas where uplands were constructed. The sand hummocks (uplands) and minimum 1 m thick tailings sand cover (low-lying areas) is covered with surficial vegetation cover soil layer made up of 0.25 m peat overlying a glacial till layer of the same thickness. The base of the mine pit was excavated into McMurray Formation which is a bitumen filled low permeability geological unit. Therefore, no significant subsurface fluxes are expected to leave the reclaimed landform through the McMurray Formation. Subsurface water transfer will be limited to the shallow subsurface through the tailings sand hummocks. Water input to the landform will be from rain and snow and water transfer out of the landform will be by evapotranspiration (ET) and overland flow at the landform outlet flowing into the closure drainage channel. The ET is controlled by the vegetation distribution over the landform. The study was limited to early reclamation timeline (first 10 years after reclamation). The uplands (hummocks) were assumed to be vegetated by treed species and the swales and low-lying areas by shrubs and wetland species. The vegetation is still being planned, but based on previous reclamation efforts of nearby landforms, uplands are likely to be vegetated with trembling aspen (Populus tremuloides Michx) and white spruce (Picea glauca (Moench) Voss) (Kessler et al., 2010; Huang et al., 2018) and wetlands with Carex aquatilis, sedges, arrow

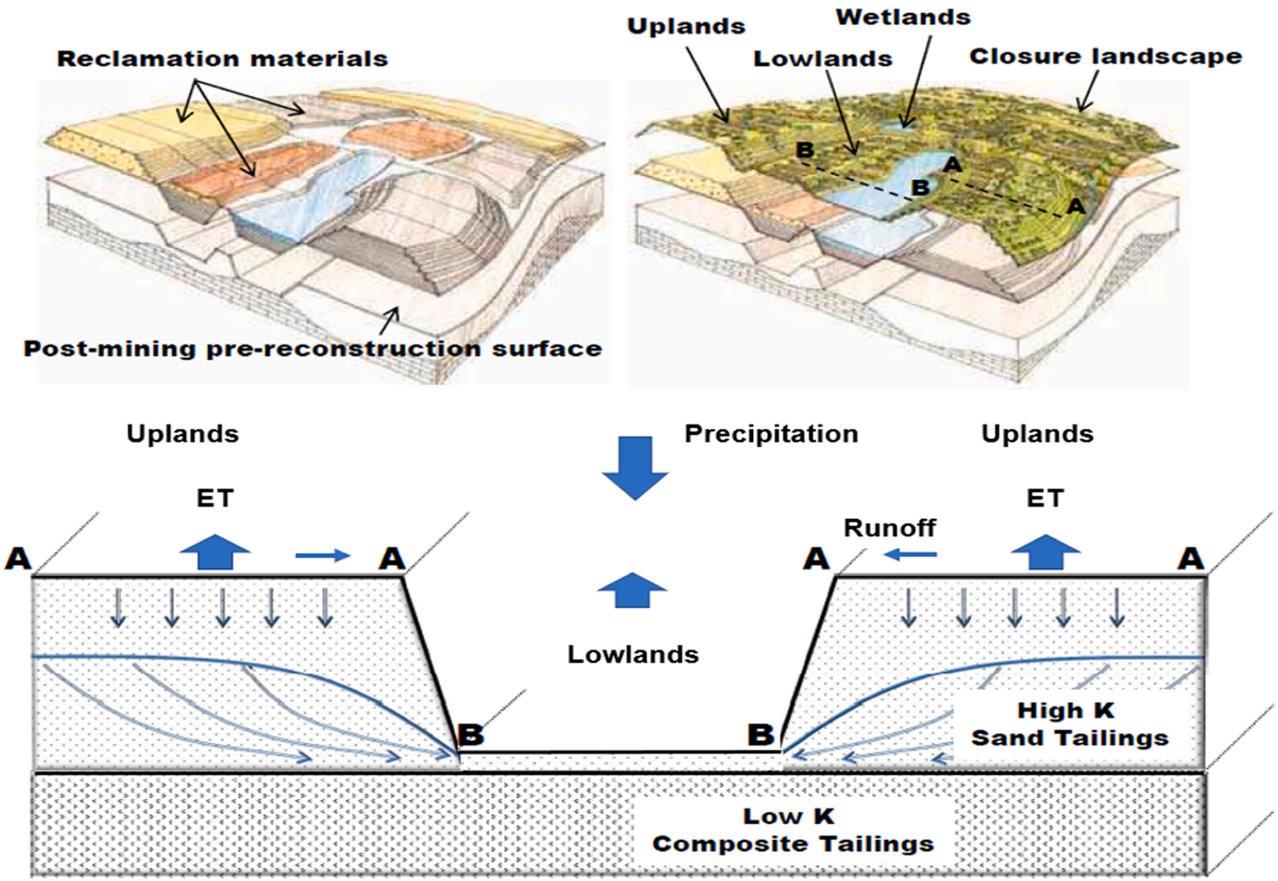

Fig. 2. Conceptual models showing post reclamation setting and key hydrological components (modified from Nagare et al., 2018).

Table 1
Model parameters.

Subsurface parameters							
Hydrostratigraphic unit	K_h (m/s)	K_h/K_v (-)	Specific storage (1/m)	Van Genuchten parameters (Van Genuchten, 1980)			
				θ_s (m^3/m^3)	θ_r (m^3/m^3)	α (1/m)	n
Soil Cover - Peat	1.8×10^{-5}	10	0.005	0.60	0.05	6.00	1.41
Soil Cover – Subsoil	3.3×10^{-5}	10	5×10^{-4}	0.36	0.02	2.80	2.22
Upper Tailings SFR > 5	1×10^{-6}	10	1×10^{-5}	0.46	0.06	2.00	4.36
Upper Tailings SFR < 5	1×10^{-8}	1	1×10^{-5}	0.41	0.05	1.12	1.25
Lower Tailings SFR > 5	1×10^{-7}	10	1×10^{-5}	0.41	0.05	1.12	1.25
Lower Tailings SFR < 5	1×10^{-9}	1	1×10^{-5}	0.36	0.05	1.12	1.25
Upper Cell Constructed Sand	1×10^{-5}	10	1×10^{-5}	0.40	0.06	2.75	8.49
Lower Cell Constructed Sand	1×10^{-6}	10	1×10^{-5}	0.35	0.06	2.75	8.49
Glacial Till	1×10^{-7}	10	1×10^{-5}	0.39	0.21	1.22	1.94
Overland parameters							
Parameter	Uplands	Lowlands	Barren Areas				
Manning's Coefficient (-)	0.09	0.05	0.03				
Rill Storage Height (m)	0.015	0.015	0.015				
Obstruction Storage Height (m)	0.01	0.01	0.01				

K_h and K_v - horizontal and vertical components of hydraulic conductivity, *SFR* - sand to fines ratio, θ_s - saturated water content, θ_r - residual water content, *α and n* - van Genuchten (1980) curve-fitting parameters.

grasses, rushes and slough grass (Ketcheson et al., 2016; Nicholls et al., 2016; Vitt et al., 2016). The precipitation is assumed to be equally distributed over the entire landform (i.e., no spatial variation). Water can flow out of the landform only when the water depth in the low-lying wetland areas exceeds the outlet elevation. The water depth in the wetland areas is determined by the interactions between the different principal components of the water budget of the landform. Precipitation inputs to the landform will be partitioned into ET, overland runoff and net percolation in hummock and swale areas (recharge). Net percolation is expected to result in flushing of the upper portion of the hummocks prior to seeping into adjacent swales and low-lying wetland areas where it mixes with overland flow (Nagare et al., 2018).

2.2. Modeling methods

HydroGeoSphere (Aquanty, 2015) was used for the 3D coupled water and solute modeling. HydroGeoSphere is a fully coupled surface water and groundwater flow, solute and heat transport model. HydroGeoSphere is also capable of modeling ground freeze-thaw processes (Schilling et al., 2019). A detailed description of HydroGeoSphere and its capabilities can be found in Aquanty (2015), Brunner and Simmons (2011), Maxwell et al. (2014) and Schilling et al. (2019). Triangular prism elements of different sizes were used to construct the 3D model grid. Each model slice in the surface and subsurface domains was discretized using 78,271 nodes and 155,640 triangular elements of different sizes. The typical hummock widths in the landform are between 150 m and 400 m, while the lengths are between 500 m and 1250 m. The typical element side length (node spacing) of 20 m or smaller was used to construct the grid. The model was discretized into 13 subsurface numerical layers of varying thicknesses. Thus, the model grid consisted of 78, 271 nodes and 155,640 triangular elements in the surface domain and 1,095,794 nodes and 2,023,320 triangular prisms in the subsurface domain. The surface and subsurface domains were separated by a coupling length of 0.001 m.

Model topography was based on LiDAR data. Model bottom elevation was based on surveyed mine bottom elevations. The bottom of the cover soil was determined by assuming a uniform 0.5 m thickness for the layer. The bottom of the tailings sand cap (i.e., top of CT layer) in the upland areas was based on the topographic survey conducted after the pit was filled with CT. The top of the CT layer rises to the level of the surrounding natural ground around the mine pit. Time-varying fluxes to represent precipitation and potential evapotranspiration boundary conditions were applied to the entire top of the model. Critical depth boundary condition was applied at the top boundary nodes corresponding to the watershed outlets to allow outflow when surface water depth exceeds ground elevation at these locations. Elsewhere, a zero gradient boundary condition was used in both the surface and subsurface domains. Details of mathematical description of the boundary conditions can be found in Aquanty (2015). Model parameters are summarized in Table 1. The CT layer was subdivided into upper and lower CT materials based on sand to fines ratios determined from cone penetration tests. Other model parameters are based on laboratory and field investigations completed by Syncrude over the years and literature values (McKenna, 2002; Shurniak and Barbour, 2002; Nagare et al., 2015a, 2018; Huang et al., 2018; Lukenbach et al., 2019; Biagi and Carey, 2020; Biagi et al., 2021).

The climatic dataset used in the model is primarily based on 1944–2020 precipitation and air temperature measured at Environment Canada's Fort McMurray Airport weather station. The long-term average annual precipitation at the station is 427 mm. The average calculated annual potential evapotranspiration for 1944–2019 period is 578 mm. The climate data shows multiple cycles of wet and dry periods, longest of which occur from 1966 to 1978 (wet cycle) and 2006–2017 (dry cycle). The recorded average annual precipitation over the wet and the dry cycles is 504 mm and 357 mm, respectively. These two periods were used to model eight (wet cycle) and seven (dry cycle) years period following reclamation assumed to be at end of year 2019. This climate input captures the highest (wet) and lowest (dry) precipitation on a decadal, annual, and daily basis. Therefore, the probability of occurrence of the estimated conditions is near a 100-year average recurrence interval (i.e., considered to have a 1% chance of occurring each year). The wet and dry climate cycle simulations were conducted with and without frozen ground processes. The model flow initial conditions

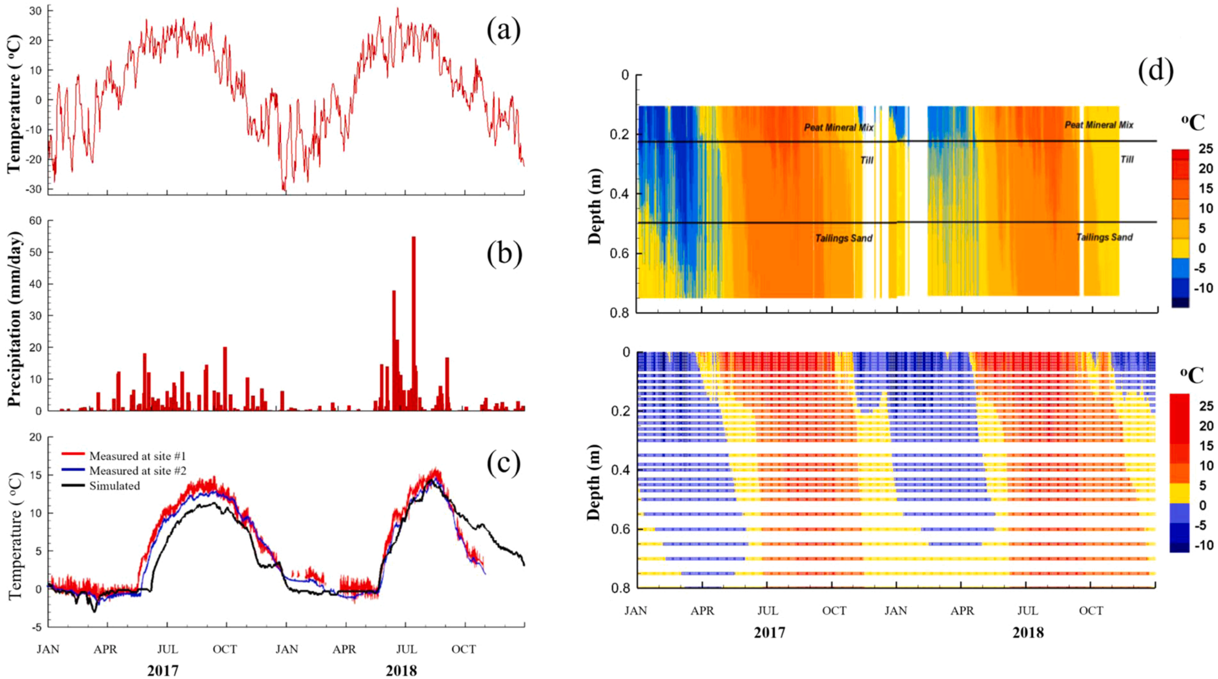

Fig. 3. Verification of the 1D hydrothermal simulations using the SHAW model: (a) air temperature and (b) precipitation at the Syncrude research sites in 2017 and 2018, (c) comparison of the measured (red and blue lines) and simulated (black line) temperature at 65 cm below ground surface, and (d) the measured (upper) and simulated (lower) time-depth-temperature distributions.

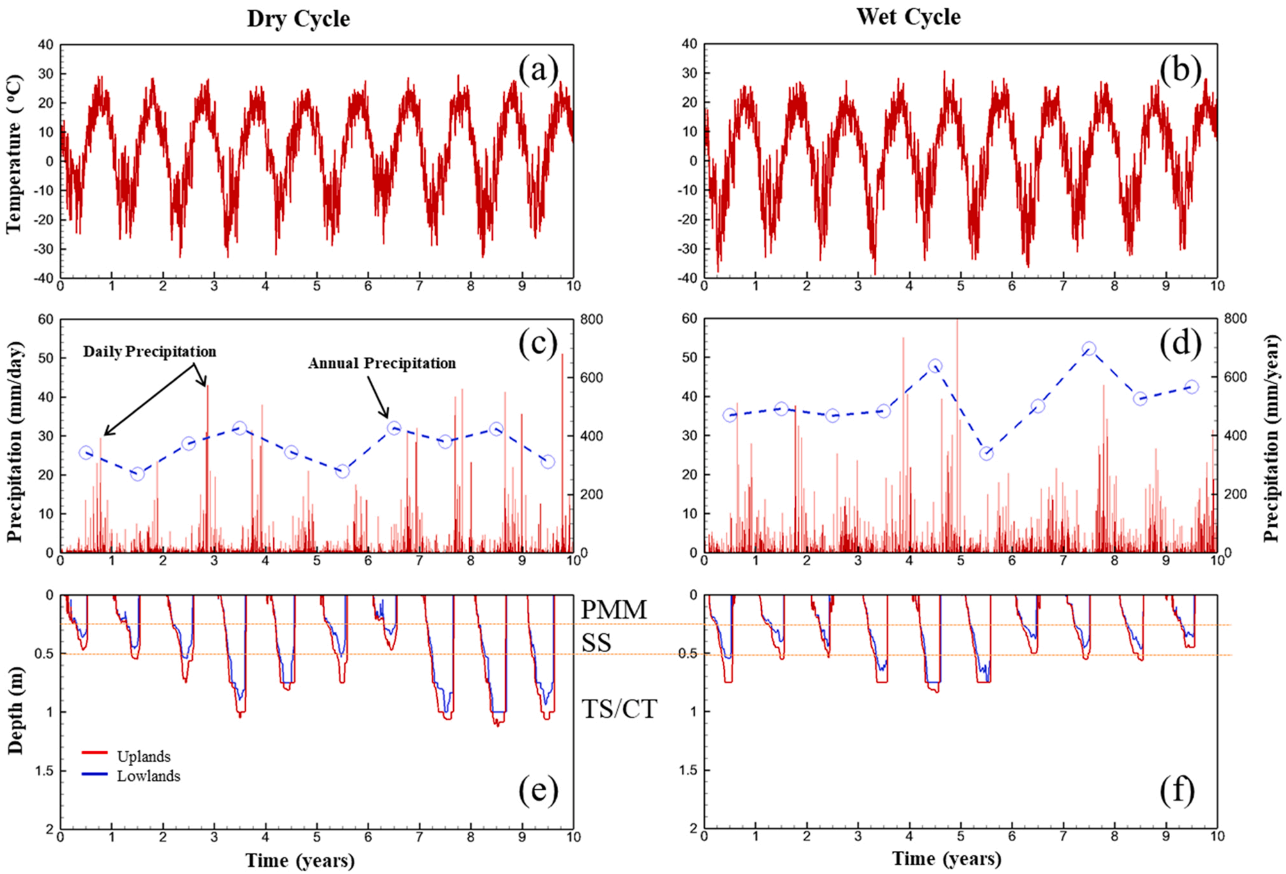

Fig. 4. Atmospheric temperature (a and b) and daily (red bars) and annual (blue dashed line) precipitation (c and d) during the first 10 years of dry (a, c, and e) and wet (b, d, and f) climate cycles used for 1D water-heat simulations. The simulated frost depth (e and f) shows that it is shallower during the wet cycle and also in the lowland areas (blue lines) due to the latent heat effects (PMM: peat-mineral mix, SS: sub-soil, TS: tailings sand in the upland areas, CT: composite tailings in the lowland areas).

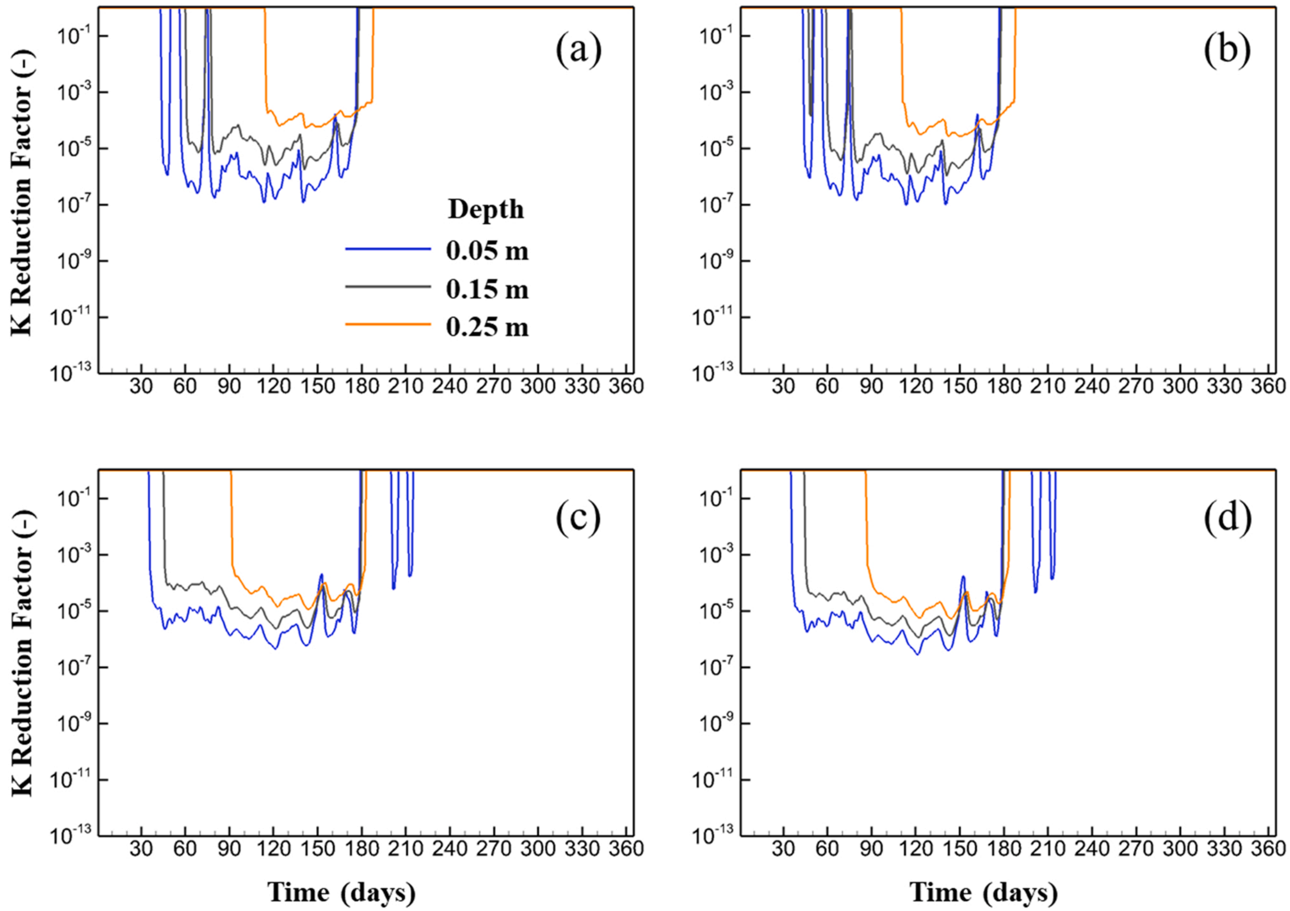

Fig. 5. Hydraulic conductivity (K) reduction factors calculated using the simulated temperature and Eq. (3) along with soil retention relations for typical dry (a and b) and wet (c and d) years and also in the lowland (a and c) and upland areas (b and d) at three different depths.

were developed by transient model spin-up using 2005–2019 climate input. Chloride transport was modeled assuming a full-strength chloride concentration throughout the reclaimed landscape based on Syncrude's tailings water quality data.

We used a hybrid approach to model the coupled water, solute and heat dynamics for this study. HydroGeoSphere is capable of simulating fully coupled water, solute and heat transfer with ground freezing and thawing if ground surface temperatures are available to be used as a boundary condition (Schilling et al., 2019). Modeling ground freeze-thaw explicitly in HydroGeoSphere along with integrated surface water and groundwater flow and solute transport, although possible, would have made the modeling computationally excessively expensive. Therefore, we used SHAW (Flerchinger and Saxton, 1989), a one-dimensional (1D) fully coupled water and heat transfer code to model the ground temperatures with freezing and thawing. We developed 1D models for upland and wetland conditions and calibrated the models to ground temperatures measured over two years at Syncrude's nearby reclamation research plot with equivalent reclamation conditions. The 1D SHAW modeling was conducted for 5 m long soil columns. The domain was discretized into 50 nodes. A 1 mm node spacing near the ground surface was gradually increased to 50 cm at the base of the column. Ground freezing and thawing reduces the effective hydraulic conductivity of the active layer (seasonally freezing and thawing zone) (Andersland and Anderson, 1978). The frost depth varies over different years depending on antecedent moisture conditions and winter air temperature. We used the daily air temperatures from Fort McMurray weather station over the modeling durations described above to model ground temperatures.

The SHAW model results are used to determine the frost depth, ice-saturation and resultant effective hydraulic conductivity of the frozen zones during freezing and thawing periods. The water potential in frozen soil (Ψ_L in J/kg), where liquid water and ice coexist, can be calculated from the absolute temperature (T in K) using the generalized form of the Clapeyron equation (Flerchinger and Saxton, 1989; Spaans and Baker, 1996; Nagare et al., 2015b).

$$d\Psi_L = (\lambda/T)dT + d\Psi_i \tag{1}$$

where Ψ_i (J/kg) is the ice potential and λ (kJ/kg) is the latent heat of fusion of water, being approximated as a function of T as:

$$\lambda(T) = -712.38 + 5.545T - 6.28 \times 10^{-3}T^2 \tag{2}$$

When the gauge pressure is assumed to be zero in the ice phase, the liquid potential can be calculated as:

$$\Psi_L = -712.38\ln(T/T_0) + 5.54(T - T_0) - 3.14\times10^{-3}(T^2 - T_0^2) \tag{3}$$

The soil retention relation, where relative permeability is a function of water potential, can then be used to determine the effective hydraulic conductivity. The hydraulic conductivity reduction due to the existence of ice or the reduction factor is used to scale the saturated hydraulic conductivity as a function of time for the 3D HydroGeoSphere simulations during freezing and thawing periods. It is noted that the transient depth of freezing and thawing zones and the hydraulic conductivity reduction factors are used in the 3D simulations as a proxy to ground freezing and thawing. Thus, hydraulic conductivity of the layers experiencing freezing and thawing is equivalent to the 1D SHAW model results in frozen zones and is internally calculated in the 3D model based on moisture content when/where layers are frost free. The above methodology is similar to the approaches used in Langford et al. (2020) and Nagare et al. (2021) to model coupled water and heat transport. This approach allows a reasonable, physically based representation of water and solute exchanges between the surface water and groundwater while overcoming the computational limitation of explicitly modeling water, solute and heat transfer with freeze-thaw in large 3D models.

3. Results and discussions

3.1. SHAW modeling

The 1D SHAW model was first verified by comparing the simulated and observed ground temperatures for two years (2017 – 2018) of reported data at two Syncrude research sites. During the two-year period, the air temperature at the research sites ranged from − 30–30 °C, with below zero being maintained for about 5 months in the winter (Fig. 3a). Precipitation was more concentrated in the summer in 2018 while it was distributed more evenly over the year in 2017 (Fig. 3b). Fig. 3c illustrates that the temperature measured at 65 cm below ground surface was similar at the two locations and the simulated temperature could reasonably reproduce the measured ground temperatures. The time-depth-temperature results shown in Fig. 3d clearly indicate that the vertical temperature profiles are strongly influenced by the material distributions at the site, especially at shallow depth where the moisture content is more responsive to the recharge events (precipitation and snowmelt). The results also show that freezing front remains mostly in the shallow cover soil zone (peat mineral mix and till layers) during most of the winter season. Freezing front penetrates below 50 cm into the tailings sand in late winter (Fig. 3d). Overall, the results indicate that the 1D water-heat model appears to be an effective alternative to a more comprehensive but computationally demanding 3D models to approximate shallow hydrothermal conditions in the study area.

The 1D SHAW model was used to analyze the hydrothermal interactions near surface under dry and wet climate conditions at the reclamation site (Fig. 4). Average daily temperatures over the first 10 years of dry and wet climate cycles show that in the wet cycle, it is slightly cooler but frost depth becomes shallower with increased precipitation and wetter ground conditions due to the latent heat effects (Fig. 4). Frost depth is generally deeper in the uplands compared to the wetter lowland area due to latent heat effects (Fig. 4e, f). Fig. 5 shows the hydraulic conductivity reduction factors at three different depths in typical dry and wet years, calculated using the simulated temperature and Eq. (3) along with the soil retention relation. The results in Fig. 5 indicate that the hydraulic conductivity can be significantly reduced in shallow subsurface during the winter months, limiting the hydrologic interactions between surface and

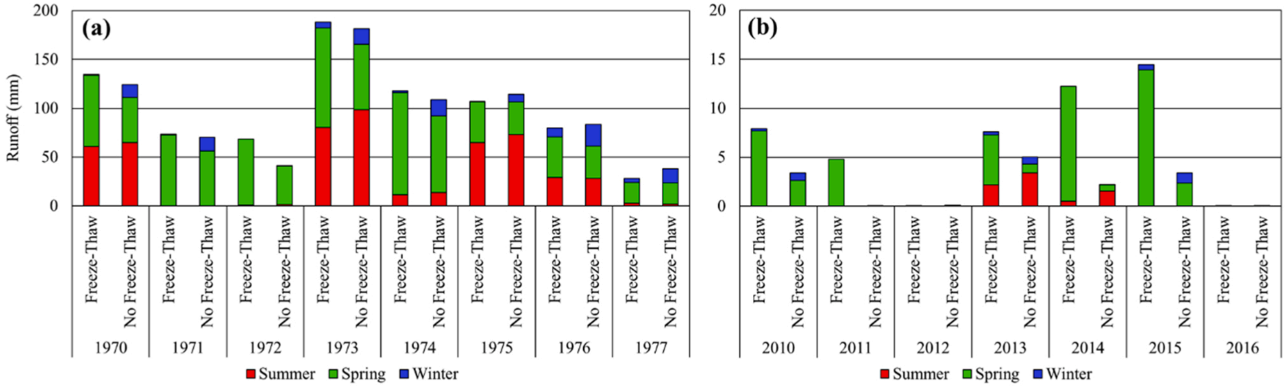

Fig. 6. Modeled outflow (mm) at the landform outlet for (a) wet climate cycle and (b) dry climate cycle. The results are stacked by seasons: summer (red), spring (green), and winter (blue). Note the difference in runoff axis scales for the two climate cycles.

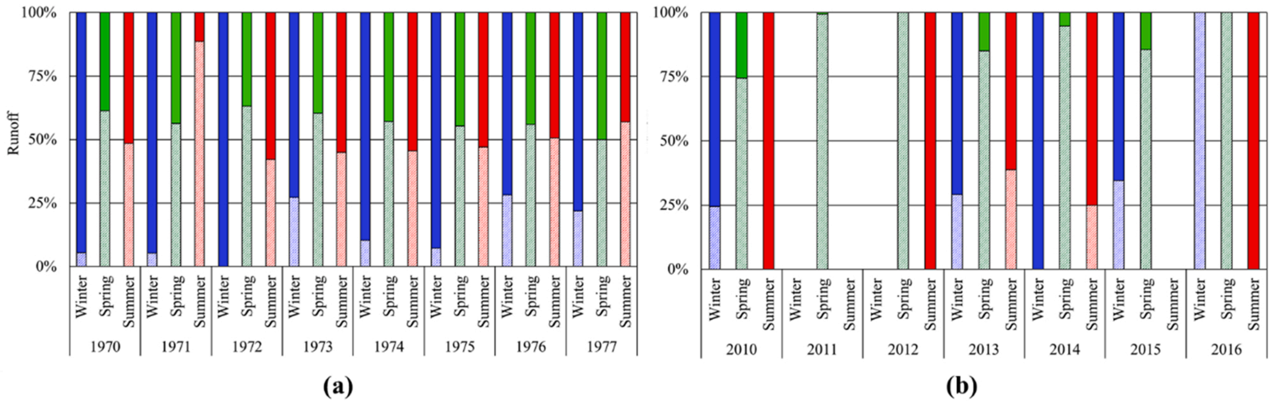

Fig. 7. Modeled outflow (%) at the landform outlet for (a) wet climate cycle and (b) dry climate cycle. The results are stacked by simulation type (i.e., with (solid colors) and without (patterned) ground freezing and thawing).

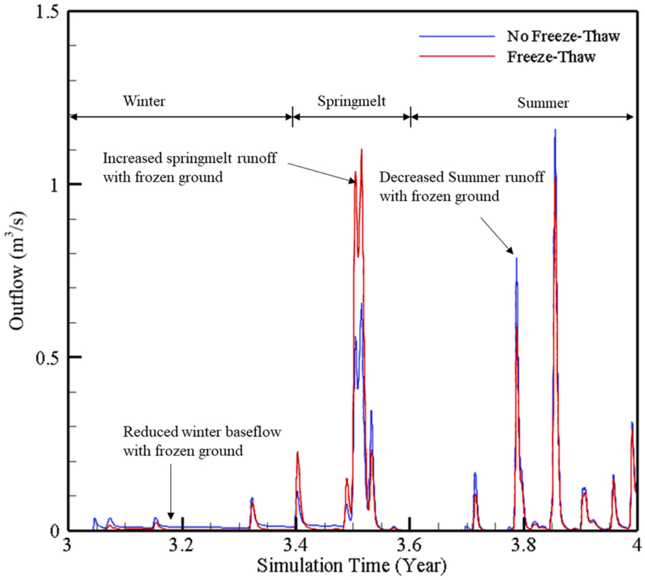

Fig. 8. Runoff hydrograph for simulations with and without frozen ground for a wet climate cycle year.

subsurface.

3.2. HydroGeoSphere model verification

A full model calibration of the 3D HydroGeoSphere was not possible as the in-pit landform is not yet fully built and long-term monitoring dataset is not available. Therefore, the model performance was verified for available data from within the partially built landform and based on data from regional natural and reclaimed watersheds. Groundwater elevations in a research plot (Twerdy, 2019) and other areas within the partially built landform are available for a limited time period. The measured and simulated groundwater table elevations matched within 2 m for the period of measurements. Seepage flux measurements from toe drains within the dykes of the partially built landform were also available. The modeled seepage rate of 6.4 L/s agrees reasonably with the measured seepage rate of 5.3 L/s. Measured actual evapotranspiration (AET) data from an adjoining reclaimed overburden dump is available for 2003–2015 period (Huang et al., 2018). The two landforms are different in characteristics and therefore not directly comparable. The modeled AET for 2010–2015 period of 354–400 mm is fairly comparable to the measured 370–450 mm range with a mean absolute and root mean squared errors of 24 mm and 27 mm, respectively.

3.3. Three-dimensional coupled water, solute and heat simulations

The 3D coupled water flow and chloride transport simulations with and without ground freeze-thaw were compared based on annual and seasonal water and chloride mass release at the landform outlet, and timing of runoff generation.

3.3.1. Water outflow

The modeled outflow is reported as depth in mm over the area of the reclaimed watershed, which can be compared easily relative to the precipitation. The model results for the wet climate cycle (Figs. 6a and 7a) suggest that annual runoff depths are 10 mm smaller (6% decrease) to 28 mm greater (67% increase) for simulations with frozen ground than without frozen ground. The average increase in runoff over the eight years of the wet cycle is 4 mm. The total runoff over the eight years is 36 mm greater (5% increase) when the simulations include frozen ground. For the dry climate cycle (Figs. 6b and 7b), the model results suggest that frozen ground conditions lead to an increased runoff for each year (0–11 mm increase), although the runoff magnitude is much smaller than the wet cycle. The total runoff over the seven-year dry cycle simulation is more than three times higher with ground freezing (47 mm vs. 14 mm). Overall, the model results suggest that the difference in annual water balance is not significant with and without heat dynamics. This is similar to the findings of Huang et al. (2018).

It is noted, however, that annual runoff alone may not provide a complete picture of the effects of frozen ground on oil sands mine reclamation. Figs. 6, 7 and 8 clearly demonstrate the effects of frozen ground on seasonal distribution of outflow. For each year of the wet and dry climate cycles, the runoff increases during spring melt season while decreasing over winter and summer seasons when ground freezing and thawing is included in the model simulations. For the eight years of the wet cycle, the winter and summer runoffs decrease by 78% and 11%, respectively, while the spring melt runoff increases by 40% (Fig. 7a). For the dry climate cycle, the outflow is distributed 18%, 46% and 36% over winter, spring melt and summer seasons when modeled without ground freezing and thawing. With ground freeze-thaw included in the model simulations, 92% of the outflow takes place during the spring season. The seasonal

Table 2
Season percentage of total outflow for wet and dry climate cycles.

Season	Wet Climate Cycle		Dry Climate Cycle	
	Freeze-Thaw	No Freeze-Thaw	Freeze-Thaw	No Freeze-Thaw
Winter	3%	14%	2%	18%
Spring	66%	49%	92%	46%
Summer	31%	37%	6%	36%

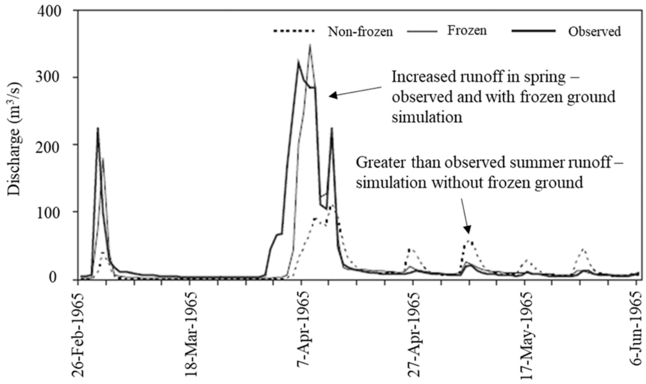

Fig. 9. Effect of frozen ground on runoff dynamics (Koren et al., 2014).

changes to outflow due to ground freezing and thawing over eight and seven years of wet and dry climate cycles are summarized in Table 2. This redistribution of outflow from the reclaimed landscape has implications for solute mass release. This information is critical for decision makers to consider because water quality is the primary criteria for the success of oil sands mine reclamation and site closure.

The reduction in outflow during the winter season is attributed to decrease in groundwater discharge (baseflow) due to freezing of surface in swales and low-lying areas. This is consistent with observations in natural systems (e.g., Wang, 2019) and in reclaimed wetlands (e.g., Ketcheson et al., 2017). The reduction in summer outflow is accounted for by relatively deeper groundwater table in the low-lying areas during the summer months, i.e., relatively increased infiltration in summer. This occurs because without ground freeze-thaw, a substantial amount of spring melt infiltrates the ground in the wetland areas and leads to increase in groundwater table. This leads to increased groundwater discharge and increased outflow during summer precipitation events. When frozen ground is incorporated in the model, relatively increased portion of spring melt is converted into overland flow while reducing the amount of infiltration. This results in deeper groundwater table in the low-lying areas at the end of spring. Consequently, more water infiltrates the ground in summer reducing the amount of outflow. This is consistent with observations in natural systems (Fig. 9, Koren et al., 2014) and in reclaimed landforms (e.g., Ketcheson and Price, 2016a; Biagi and Carey, 2020).

3.3.2. Solute mass release

Salt is a constituent of interest for reclamation planners in Alberta's oil sands region. Long-term effects of salinity on vegetation growth and end pit lake water quality (sustainability) are currently being studied. This study is part of advancing the knowledge on quantifying salt release from reclaimed landforms. Chloride was used as a proxy for salt concentrations in the water cycling within the landform and in the outflow from the landform. The model results suggest that there is approximately a 20% reduction in chloride mass release over the wet cycle when ground freezing effects are considered (Figs. 10a and 11a). The reduction in chloride mass release is a direct result of decreased baseflow in winter, increased spring melt runoff and decreased outflow in summer. The decrease in winter baseflow and summer outflow results into reduced chloride transfer from uplands to lowlands in simulations with ground freezing and thawing. This is critical since this improves the water quality for wetland vegetation. The 20% reduction in eight wet years is a significant reduction in solute load to the end pit lake. In addition, the end pit lakes receive fresher water in spring melt season. The spring melt outflow chloride concentrations for simulations with freeze-thaw reduce by a factor of 1.1–1.6 (Fig. 12) over the eight years when compared to simulations without freeze-thaw. The summer outflow chloride concentrations remain unchanged, but 11% lesser outflow results into reduced chloride mass release. This is an important insight towards assessing the sustainability of the end pit lakes and overall success of oil sands mine reclamation.

The chloride mass release during the dry cycle is generally an order of magnitude smaller than the mass release during the wet cycle (Figs. 10b and 11b) primarily due to the reduced runoff (Fig. 6b). As discussed above, the outflow increases during the dry cycle when frozen ground is included in the simulations (47 mm vs. 14 mm). This is primarily due to the increased spring melt contribution. The spring melt outflow concentrations for simulations with freeze-thaw reduce by a factor of 1.1–1.7 over the seven years when compared to simulations without freeze-thaw. The total chloride mass release over the seven-year dry cycle simulation increases by 2.3 times

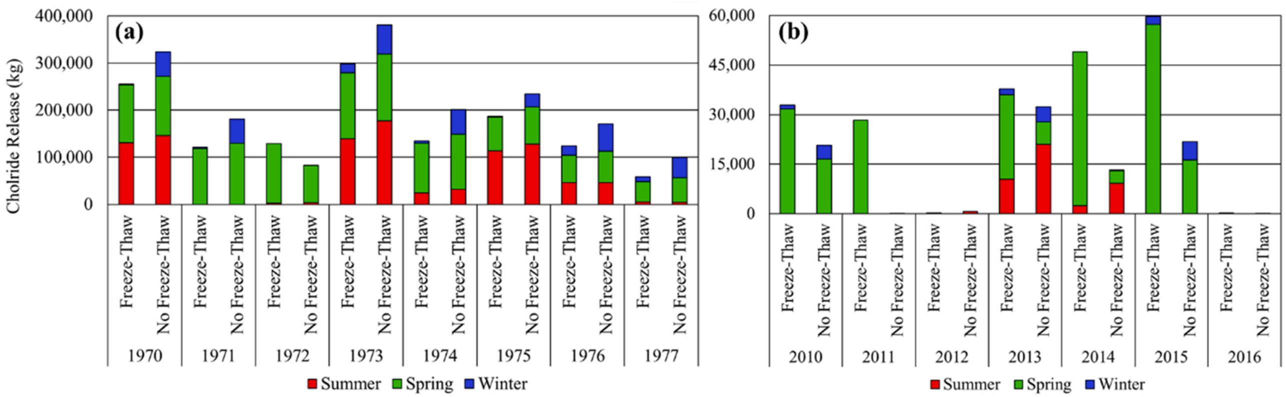

Fig. 10. Modeled chloride mass release at the landform outlet for (a) wet climate cycle and (b) dry climate cycle. The results are stacked by seasons (summer, spring, winter). Note the difference in chloride release axis scales for the two climate cycles.

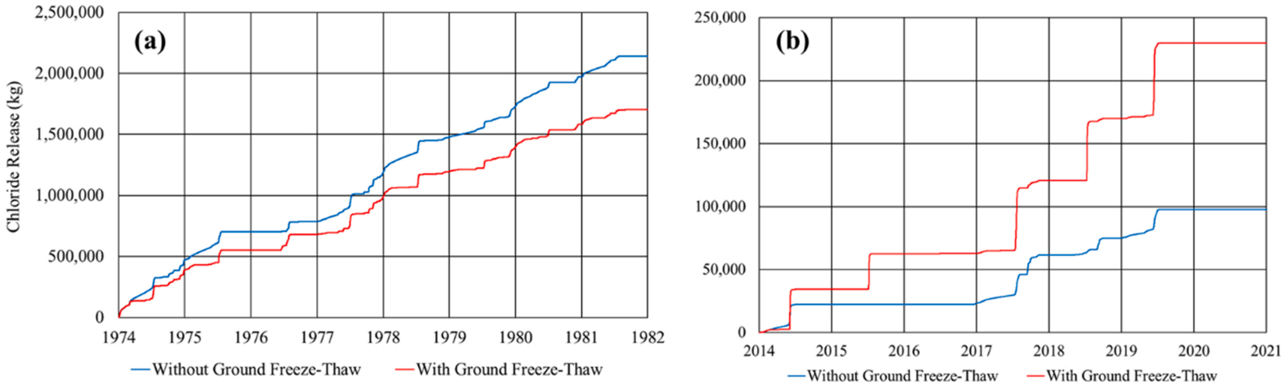

Fig. 11. Modeled cumulative chloride mass release at the landform outlet for (a) wet climate cycle and (b) dry climate cycle. Note the difference in chloride release axis scales for the two climate cycles.

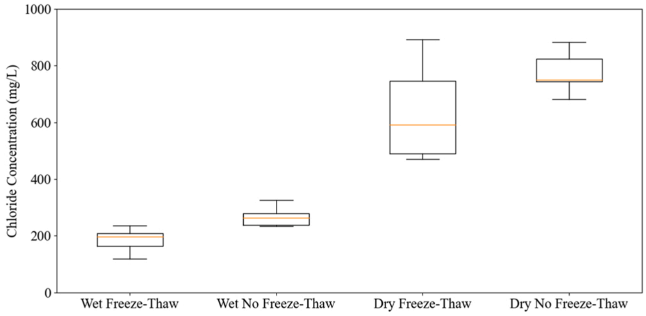

Fig. 12. Modeled chloride concentrations in outflow for different simulations.

(208,000 kg vs. 89,000 kg) for simulations with freeze-thaw. However, this is not significant since majority of the water and solutes are flushed during wet years. In terms of oil sands reclamation success, the increased outflow in dry years is important as additional water flowing to the end pit lakes offsets the lake evaporation. The increased outflow of salt due to frozen ground during the dry cycle is beneficial because it reduces the potential for evapoconcentration and improves water quality in the low-lying wetland areas of the reclaimed landform.

4. Summary and conclusions

This study presents an integrated surface water and groundwater modeling approach to evaluate performance of oil sands mine currently being reclaimed. The modeling includes most important hydrological and solute transport processes while maintaining a reasonable balance between inclusion of details of the processes, and computational cost and parameterization effort. We coupled a physically based three-dimensional (3D) integrated surface water and groundwater flow and solute transport model with a fully coupled one-dimensional (1D) heat and water transfer model. Specifically, we included changes to hydraulic conductivity of the near surface materials in the 3D model due to freeze-thaw based on the results of the 1D model. This approach allows for reasonably simulating effects of frozen ground on infiltration and overland runoff processes.

The modeling provided estimates of differences in outflow and chloride mass release from the reclaimed landform when simulated with and without frozen ground. The model results suggest that outflow from the reclaimed landscape would occur only during wet years. Annual water balance comparisons for transient simulations with and without coupled heat dynamics is almost identical. Inclusion of frozen ground leads to increased runoff in wet and dry years, however the magnitude of outflow in dry years is comparatively small. The 3D representation of ground freeze-thaw led to reduced infiltration during spring melt, deeper groundwater table in the low-lying areas during summer and reduced salt loading during winter. Chloride mass released from the reclaimed landscape is reduced by 20% over eight-year wet climate simulation with frozen ground. This reduction is a result of 11% and 78% decrease in summer and winter outflows, respectively. Winter outflow reduction is due to delayed groundwater seepage due to ground frost in wetlands. This is consistent with observations of Ketcheson et al. (2017) and Wang (2019) for reclaimed and natural systems, respectively. Spring melt runoff for wet climate model simulation with frozen ground increases by almost 40% as compared to model simulation without frozen ground. This simulation result is consistent with observations of Ketcheson and Price (2016a) and Biagi and Carey (2020) for reclaimed landforms and Koren et al. (2014) for natural systems. Together, the decrease of outflow in winter and increase of freshwater flow in spring season results in reduction of outflow chloride concentrations by a factor of 1.1–1.6 for the two seasons. Summer outflow chloride concentrations remain unchanged during the wet cycle, however 11% reduction in outflow leads to reduced mass release.

Overall, the seasonal partitioning of outflow and salt loading with ground freeze-thaw suggests that the effects of frozen ground are significant. The increased volume and fresher water quality discharge to the end pit lakes is beneficial for sustainability of end pit lakes during wet and dry cycles. Including ground freeze-thaw in integrated surface and groundwater models is computationally intensive. The results of this work suggest that previous models that did not include ground freeze-thaw are conservative since water quality is expected to improve with inclusion of ground freeze-thaw effects. This work would allow decision makers in the oil sands industry to better assess model results and understand the conservatism in outflow and solute mass release results when not including ground freeze-thaw.

The modeling approach developed in this study was able to successfully simulate the differences in water balance and water quality responses within the reclaimed landform. At the same time, the modeling approach provided a practical modeling framework to incorporate ground-freeze thaw and winter hydrological processes without excessively increasing the computational burden of the integrated model. The model reasonably captured the landform scale seasonal hydrological responses; however, it is acknowledged that local scale processes were simplified in order to reduce the parameterization burden. For example, the 1D coupled heat and water transfer models were developed only for representative upland and wetland/lowland in a landform that is made up of several upland hummocks draining to the low-lying areas through a series of swales. It is possible that ground-freeze thaw timing within different hummock uplands is not the same, which was not necessarily captured in the modeling described in this paper. This can be improved in future studies once more data from the landform is collected.

The 3D model results suggest that the implications of coupled heat dynamics should be considered when performing detailed evaluation of reclaimed in-pit oil sands landforms where detailed evaluation of reclaimed in-pit landforms at finer time scales is desired. The results also suggest that modeling in-pit tailings landforms without freeze-thaw provides a conservative estimate of solute release and reasonable water balance on an annual basis, which is appropriate for coarse site-wide models.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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