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Towards the incorporation of hydrogeochemistry into the modelling of permafrost environments: a review of recent recommendations, considerations, and literature

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Abstract

This study is a meta-analysis of recent global research articles on hydrogeochemical modelling of permafrost regions to determine trends and consensus on research gaps and future research directions. The hydrogeochemical response of permafrost to climate change remains challenging to estimate and forecast despite evidence of large-scale impacts on freshwater and ecological cycles. We investigate the feasibility, need, and potential for hydrogeochemical modelling of permafrost landscapes by reviewing recommendations from previous modelling, review, and primer papers, including discussing ways to advance this type of modelling science. Key permafrost hydrogeochemical processes are discussed, including heat transfer and associated freeze–thaw regimes, biogeochemical processes and rates, and surface and subsurface flow. Modelling considerations (i.e., model dimension, scale, heterogeneity, and permafrost zonation) and model parameters are subsequently examined. Finally, limitations and additional considerations for advancing permafrost hydrogeochemical modelling efforts are reviewed. The findings of this review are summarized in recommendations, tables, and two schematics incorporating key considerations for future hydrogeochemical modelling initiatives in permafrost environments.

Key words: permafrost, permafrost hydrology, hydrogeochemistry, modelling, climate change

1. Introduction

Permafrost, ground that remains at or below 0 °C for two or more consecutive years and may or may not contain ground ice (van Everdingen 1998), is increasing in temperature and is thawing unevenly across the circumpolar north in response to an interplay of factors, including climatic changes (Smith et al. 2022). However, it is unclear how cold region hydrology will respond to climate change as permafrost stability depends on several physical and chemical factors. This, combined with a poor understanding of how to represent crucial physical processes in models (Elshamy et al. 2020), results in major challenges in predicting climate change impacts (Jorgenson et al. 2010). In turn, natural hydrogeochemistry is also expected to experience climate-related impacts. Dissolved organic carbon (DOC), nutrients, and other ionic fluxes are changing and predicted to accelerate in permafrost environments (Striegl et al. 2005; Petrone et al. 2006; Frey and McClelland 2009; Abbott et al. 2015), with hydrogeochemical process rates changing through altered vegetation, increased permafrost and seasonal thaw, earlier snowmelt, increased rain (Shatilla and Carey 2019), water temperature changes (Todd et al. 2012; Barkow et al. 2021), and groundwater discharge to major rivers (Walvoord and Striegl 2007). Permafrost influences hydrogeochemistry by influencing the subsurface material through which water flows (Walvoord and Kurylyk 2016) and therefore influences stream flow geochemistry (Petrone et al. 2006; Bagard et al. 2011), nutrient seasonal fluxes (Frey et al. 2007; Frey and McClelland 2009), solute fate (Mohammed et al. 2021*a*), subsurface flow paths (Walvoord and Kurylyk 2016), and residence times in soil (Frampton and Destouni 2015) and impedes groundwater recharge (Cochand et al. 2019), subsequently impacting aquatic chemical exports (Striegl et al. 2007; Walvoord and Striegl 2007; Vonk et al. 2015). A better understanding and quantification of permafrost change and its effects on hydrogeochemical regimes is critical to anticipate how Arctic hydrology and associated stream solute exports may be affected, and how it may impact freshwater and coastal ecosystems (Wrona et al. 2016). Further, knowledge of natural hydrogeochemistry is essential in permafrost-degrading regions where water resources may be used for personal or industrial use (Cochand et al. 2019). Even with the existing knowledge as summarized above, there is a limited capability to predict the hydrogeochemical impacts of permafrost response to climate change at reach and watershed scales (Andresen et al. 2020), resulting in a need for tools that help identify control mechanisms and key hydrogeochemical processes in changing permafrost environments.

2. Review motivation and structure

Overlapping knowledge and research gaps exist in the modelling of hydrological and hydrogeochemical processes, including groundwater flow (Walvoord and Kurylyk 2016; Piovano et al. 2019; McKenzie et al. 2021; Mohammed et al. 2021*a*) and the quantification of subsurface (Lafrenière and Lamoureux 2019; McKenzie et al. 2021) and lateral flow paths and transport (McGuire et al. 2018; McKenzie et al. 2021). Although many hydrological models exist, they are not easily transferable to permafrost environments for several reasons, including the seasonality of discharge and flow pathways (Douglas et al. 2013) and water phase transformation and associated energy balances of solid, liquid, and vapour phases (Gao et al. 2021). Simultaneously, climate models show biases in estimating many hydrological variables at high northern latitudes because of missing processes and associated deficiencies in land surface schemes that are used to couple atmospheric and hydrological models (Swenson et al. 2012). Permafrost hydrogeochemical modelling can help assess changes in these environments; however, the uncertainties associated with hydrological modelling can result in difficulty in creating reliable models for hydrogeochemical processes (e.g., Douglas et al. 2013). Moreover, large research gaps exist in multiple components directly associated with the hydrogeochemical response to permafrost change, including (1) the biogeochemical impacts of subsurface hydrological processes (Lafrenière and Lamoureux 2019; McKenzie et al. 2021); (2) reactive solute transport dynamics and routines (Mohammed et al. 2021*a*); (3) the pathways, flow dynamics, and associated processes responsible for solute, nutrient, and carbon (C) transport (McGuire et al. 2018; Cochand et al. 2019; Lafrenière and Lamoureux 2019; Vonk et al. 2019; Bowring et al. 2020; Walvoord and Striegl 2021); (4) the determinants of fate and lability of organic carbon (Lafrenière and Lamoureux 2019); (5) the effect of changing nutrient and carbon export seasonality and river geochemistry (Douglas et al. 2013); and (6) existing solute transport models do not typically include permafrost dynamics (Mohammed et al. 2021*a*). Therefore, coupled cryohydrogeological and biogeochemical modelling approaches are required to better constrain the fate of permafrost-sequestered C, nitrogen (N), and mercury (Hg) (Walvoord et al. 2019) and other hydrogeochemical processes in changing permafrost landscapes.

Here, we investigate the feasibility, need, and potential for hydrogeochemical modelling of permafrost landscapes by reviewing recommendations and results from recent (i.e., 2008 onwards) modelling, review, and primer studies (see following sections) to help guide and advance future research efforts. We review studies that relate to the incorporation of hydrogeochemistry modelling into permafrost environments using the best possible type of model. As such, we did not exclusively review permafrost modelling studies. Instead, we reviewed various studies that used different hydrological, permafrost, climate, and geochemical models. In Section 3, we discuss relevant background information pertaining to hydrogeochemistry in permafrost environments in further detail. This provides the proper context for our review of recent hydrogeochemistry modelling studies and reviews relevant to permafrost environments in Section 4 and the subsequent discussion of considerations for modelling hydrogeochemistry in permafrost environments in Section 5. The findings of this review are summarised in two figures and several tables that incorporate critical considerations for future hydrogeochemical modelling efforts in permafrost environments, coupled with key recommendations and takeaway messages concluding the review in Section 6.

3. Hydrogeochemistry of permafrost environments

Permafrost has a heterogeneous circumpolar distribution and is divided into different zonations based on the percentage of ground underlain by permafrost in the region: continuous, discontinuous, sporadic, and isolated patches (Brown et al. 1997). The presence of permafrost has a profound influence on surrounding hydrological processes. The physical and thermal regime of permafrost (Carey and Woo 2001; Lafrenière and Lamoureux 2019), cryostratigraphy (Carey and Woo 2001; Lafrenière and Lamoureux 2019), and active layer dynamics (Lafrenière and Lamoureux 2019) dictate key water parameters, including its flow paths (Carey and Woo 2001), routing, storage, drainage, and surface and subsurface distribution (Andresen et al. 2020). In many cases, permafrost can behave as an impermeable layer preventing vertical water flow, subsequently resulting in saturated near-surface soil conditions (Hagemann et al. 2014; Walvoord and Kurylyk 2016; Liao and Zhuang 2017) and often constraining subsurface flow to perennially unfrozen ground (e.g., taliks) (Walvoord and Kurylyk 2016). These saturated zones of permafrost cryostratigraphy are important, as wetter soil is characterized by increased thermal conductivity (Grant et al. 2019) and heat capacity (Walvoord and Kurylyk 2016). Hydrological flow paths in permafrost environments exist at the topographic surface and in suprapermafrost, intrapermafrost, and subpermafrost aquifers (Woo 2012; Cochand et al. 2019), with water movement dependent on parameters including hydraulic conductivity of the ground and associated hydraulic gradients (Walvoord and Kurylyk 2016).

Hydrological effects associated with permafrost change (e.g., thermokarst, degradation, and thaw) can be thermal, physical, or biogeochemical. Thermal perturbation is used to describe a change in soil and active layer extent, while physical perturbation (or disturbance) is used to describe the process where surface materials are altered, resulting in changes to the active layer's physical properties. Surficial changes to permafrost are seen through thaw slumping, thermo-erosional gullying, and slope disturbances (Lafrenière and Lamoureux 2019). Permafrost thaw can occur (1) downwards with increasing active layer thickness; (2) internally as a result of groundwater intrusion (Jorgenson et al. 2010); (3) laterally as a result of heat transported with ground and surface water (Jorgenson et al. 2010; Devoie et al. 2021); and (4) upwards from the geothermal heat flux (Jorgenson et al. 2010; Dagenais et al. 2020) and advective heat transfer from subpermafrost groundwater flow (Dagenais et al. 2020). Permafrost zonation dictates the hydrological effect of thaw. For example, shallow permafrost thaw processes influence hydrological and C cycles in continuous permafrost environments, including active layer deepening and thermokarst presence/formation. In contrast, deeper permafrost thaw processes such as suprapermafrost talik development and permafrost loss have larger impacts in discontinuous permafrost zones (Walvoord and Striegl 2021).

Hydrogeochemistry can be characterised using major ions, stable isotopes, and nutrients (Cochand et al. 2019), with solute fate driven by a complex interplay between biotic and abiotic processes, residence time, hydrological transport within aquatic–terrestrial environments (Wickland et al. 2018), and soil/rock interactions (Zhang et al. 2016). The geochemistry of permafrost is largely associated with permafrost history and ice formation processes (Paquette et al. 2022). The variability of geochemical constituents such as soluble ion distribution (Woo 2012), stored organic carbon (Kuhry et al. 2010), and DOC concentrations (Kicklighter et al. 2013) makes it useful to consider hydrogeochemical processes using permafrost cryostratigraphy (Lafrenière and Lamoureux 2019) (i.e., the frozen layers in the ground; French and Shur 2010) and permafrost zonation. If permeable, the seasonally thawed active layer above the permafrost controls isotope and nutrient cycling (Koch et al. 2013; Tetzlaff et al. 2015), changes in water quality (Lafrenière and Lamoureux 2019), and DOC production and export timing (Kicklighter et al. 2013). Many hydrogeochemical processes in the continuous permafrost zone occur in the active layer (Fabre et al. 2017), with the potential for increased solute mobilization with permafrost thaw (Paquette et al. 2022). Suprapermafrost groundwater is characterised by low mineralisation levels and short residence times, with its hydrogeochemistry affected by precipitation composition, mineralogical composition, and the distance from recharge zones (Cochand et al. 2019). The downward migration of the freezing front through the active layer can fractionate some solutes and soil water nutrients downward (Douglas et al. 2013). This transient layer of permafrost is impacted by freeze–thaw transitions over longer timescales and can join either the active layer or the top of permafrost at a given time (Shur et al. 2005). This layer is therefore characterised by either the persistence of liquid water (Walvoord and Kurylyk 2016) or high ice content and by varying nutrient and solute composition (Kokelj and Burn 2003; Shur et al. 2005; Lamhonwah et al. 2017), and it is considered a source of dissolved species following substantial perturbation (Lafrenière and Lamoureux 2019). Near-surface permafrost soils can be equally important contributors of DOC and total dissolved nitrogen (TDN) (Wickland et al. 2018), with C and N stocks found in this layer (Harden et al. 2012). The cryopeg at the base of permafrost also allows the persistence of liquid water (Walvoord and Kurylyk 2016). Water can be present in permafrost, though ice-rich permafrost often has reduced hydraulic conductivity and soil/rock porosity (Cochand et al. 2019). Hydrogeochemical flow paths in continuous permafrost are influenced by talik origin (Cochand et al. 2019), the organic layer, rainfall events (Sjöberg et al. 2021), and fractures in the associated rock or sediment (Hornum et al. 2021). In contrast, the discontinuous permafrost zone is vulnerable to enhanced subsurface connectivity (Vonk et al. 2019; Devoie et al. 2021), resulting in more ubiquitous hydrogeochemical flow paths (Cochand et al. 2019).

Permafrost change impacts hydrogeochemistry by changing groundwater recharge zones and flow and transport pathways (Cochand et al. 2019; Shatilla and Carey 2019), including those carrying dissolved organic matter (DOM) (Shatilla and Carey 2019), particulate matter (Lafrenière and Lamoureux 2019), previously frozen carbonates in permafrost (Walvoord and Striegl 2021), and phosphorus (Shogren et al. 2019). Specifically, permafrost thaw will (1) allow the mobilisation of major ions, contaminants, sediments, nutrients, and organic matter (Vonk et al. 2015); (2) increase nutrient and inorganic solute export (Petrone et al. 2006; Roberts et al. 2017; Lafrenière and Lamoureux 2019; Connolly et al. 2020; Zolkos et al. 2022) through availability for leaching (Treat et al. 2016; Lafrenière and Lamoureux 2019) or biogeochemical transformation (Lafrenière and Lamoureux 2019); (3) increase longitudinal and lateral solute flux in aquatic and terrestrial ecosystems (McClelland et al. 2016); (4) impact in-stream processing by increasing DOC oxidation potential (Ward et al. 2017) and the photodegradation of thawing permafrost DOM and organic mat DOM (Ward and Cory 2016) in surface waters; and (5) affect reaction and dissolution rates, ion exclusion, and gas hydrates (Cochand et al. 2019).

4. Review and modelling papers relevant for hydrogeochemical modelling of permafrost environments

Several recent review papers have synthesised current research on hydrology and associated modelling in permafrost environments and are important when considering the feasibility of hydrogeochemical monitoring in permafrost regions. These papers have reviewed (1) permafrost hydrology (Walvoord and Kurylyk 2016; Lafrenière and Lamoureux 2019) and geomorphology (Lafrenière and Lamoureux 2019); (2) permafrost hydrological (Walvoord and Kurylyk 2016; Bui et al. 2020; Gao et al. 2021) and land (Andresen et al. 2020) models; (3) impacts of permafrost thaw on aquatic systems (Vonk et al. 2015), including aquatic C cycle vulnerability (Walvoord et al. 2019) and material aquatic release and transport from permafrost (Tank et al. 2020); (4) DOC modelling and dynamics in permafrost environments (Ma et al. 2019); and (5) groundwater hydrogeochemistry in permafrost environments (Cochand et al. 2019). Table 1 provides a summary of these relevant review papers.

Few modelling studies have focused on hydrogeochemical processes in permafrost environments. Studies that incorporate a geochemical modelling component focus predominantly on carbon dynamics (i.e., Yurova et al. 2008; Kicklighter et al. 2013; Lessels et al. 2015; Bowring et al. 2020; Yi et al. 2020; Pongracz et al. 2021) and do not include

Table 1. Recent (2015 onwards) review papers that synthesize current research on hydrology and associated modelling in permafrost environments that are important when considering the feasibility of hydrogeochemical monitoring in permafrost regions.

Authors	Relevant review topic(s)	Additional contribution(s)	Permafrost zonation
Vonk et al. (2015)	• Impacts of permafrost thaw on aquatic ecosystems, including physical, optical, and chemical limnology changes, and terrestrial materials release to water		Multiple
Walvoord and Kurylyk (2016)	• Permafrost hydrology and hydrological impacts of climate warming • Recent improvements in hydrological monitoring in permafrost environments • Impacts of permafrost distribution on surface and subsurface routing		Discontinuous
Cochand et al. (2019)	• Current knowledge of groundwater hydrogeochemistry in permafrost environments		Multiple
Ma et al. (2019)	• DOC modelling and dynamics in permafrost environments		Multiple
Lafrenière and Lamoureux (2019)	• Permafrost hydrology and geomorphology		Continuous
Andresen et al. (2020)	• Common permafrost-enabled land models in northern permafrost regions • Research gaps and difficulties simulating permafrost hydrology		Multiple
Bui et al. (2020)	• Assessing hydrological model suitability for simulating Arctic hydrological processes		Multiple
Tank et al. (2020)	• Analysis of case studies and summary of recent progress in material aquatic release and transport from permafrost	• State factor approach that predicts material aquatic release and transport from permafrost	Multiple
Gao et al. (2021)	• Current state of permafrost hydrological models for the Qinghai–Tibet Plateau and associated challenges		Multiple
Walvoord and Striegl (2021)	• Field and modelling studies investigating water and aquatic C cycle vulnerability to permafrost thaw	• Framework assessing water and aquatic C cycle vulnerability in Arctic-boreal regions	Multiple

Note: C, carbon.

subsurface hydrological pathways (i.e., Kicklighter et al. 2013; Lessels et al. 2015; Bowring et al. 2020; Pongracz et al. 2021; Yi et al. 2021*a*, 2021*b*), leaving other hydrogeochemical constituents and subsurface and lateral hydrological modelling largely absent from the existing permafrost hydrogeochemical modelling literature. For example, the modelling of lateral hydrological C flux response to permafrost change is largely omitted or simplified in large-scale models (Ala-aho et al. 2018; Hugelius et al. 2020; Tank et al. 2020), with no models known to simulate the lateral flow of deeper groundwater C released following permafrost thaw (Ma et al. 2019). While some terrestrial ecosystem models do include N and C pools in vegetation and soil and associated soil–atmosphere–vegetation fluxes, they lack hydrogeochemical components for the permafrost subsurface (Yi et al. 2014). Three studies investigated hydrogeochemical activities in permafrost environments that included subsurface liquid water processes and focused on (1) reactive solute transport in a permafrost environment (i.e., Mohammed et al. 2021*a*); (2) the impacts of climate and permafrost change on water flow and solute transport (i.e., Frampton and Destouni 2015); and (3) quantifying potential pathways of groundwater and solute transport between Quaternary deposits and bedrock under various permafrost conditions (i.e., Bosson et al. 2013). Two studies (i.e.,Frampton and Destouni 2015; Mohammed et al. 2021*a*) employed process-based cryohydrogeological and reactive solute transport models, which are cold-region groundwater flow models that typically involve incorporating both surface and subsurface processes, in addition to freeze–thaw processes and associated impacts on ground energy balance and thermal and hydraulic characteristics (Bui et al. 2020; Lamontagne-Hallé et al. 2020). The third study employed a three-dimensional (3D) physically based, groundwater flow and transport model, MIKE SHE (Bosson et al. 2013).

Limitations from these studies included (1) a lack of active layer and permafrost data available for proper model calibration and validation (Mohammed et al. 2021*a*); (2) not simulating unsaturated (vadose) zone processes or changes in fluid density (Mohammed et al. 2021*a*); (3) missing functionality for thermal modelling (Bosson et al. 2013); and (4) the simulation of typical geological configurations instead of study-specific regions (Frampton and Destouni 2015). A summary of recent (2008 onwards) relevant examples of hydrogeochemical modelling studies related to permafrost environments is provided in Table 2.

5. Considerations for modelling hydrogeochemistry in permafrost environments

5.1. Critical processes

Permafrost hydrological, and by association hydrogeochemical, modelling requires the consideration of heat transfer processes (Walvoord and Kurylyk 2016; Grant et al. 2019) and heat fluxes (Fabre et al. 2017). Associated freeze–thaw regimes are particularly important to consider as they result in water and solute immobilization and subsequently enhance solute residence times in the active layer (Mohammed et al. 2021*a*). Freeze–thaw cycles can also result in ice expansion and soil grain displacement. These two processes can increase solute advection and dispersion and active layer hydraulic conductivity through the creation of larger pores and an increase in smaller and isolated pores (Ding et al. 2019; Mohammed et al. 2021*b*). Thaw layer dynamics are also important as they exhibit control over water routing (Bui et al. 2020) and flow paths and the biological capacity to retain and process nutrients and DOM (Harms et al. 2019). Incorporating thaw dynamics can result in more realistic model predictions (Fabre et al. 2017), yet the ground thermal regime has been highlighted as a common challenge in hydrogeochemical modelling (Kurylyk et al. 2016; Walvoord and Kurylyk 2016; Fabre et al. 2017) as its simulation is very sensitive to model parameters (Harp et al. 2016; Wu et al. 2016).

Biogeochemical processes and rates also need to be considered in hydrogeochemical modelling efforts in permafrost environments. These processes exhibit seasonality (e.g., seasonal nutrient and geochemical characteristics are largely controlled by rain (Douglas et al. 2013) or snowmelt (Hayashi 2014)). For example, DOC concentrations increase with the onset of flow events (Shatilla and Carey 2019), with the highest exports associated with shallow active layers in the early spring (Frey and McClelland 2009), and DOC becomes increasingly immobilised later in the season when the active layer deepens (Koch et al. 2013). Following winter soil freeze-up, groundwater flow originates from deeper flow paths that typically hold carbonate minerals (Douglas et al. 2013). Snow–soil–vegetation feedbacks are also important to understand to investigate climatic changes when using Arctic global-scale land surface modelling (Pongracz et al. 2021). Therefore, it is important to couple biogeochemistry (i.e., vegetation and the carbon cycle) to quantify feedbacks associated with wetlands and permafrost (Hagemann et al. 2014).

Climate change and associated impacts on permafrost can also influence hydrogeochemical processes. Physical disturbances can increase particulate and dissolved inorganic ion concentrations (Lafrenière and Lamoureux 2019) and increase inorganic N flux (e.g., Abbott et al. 2015) and plant-available N (Keuper et al. 2012). Thermokarst, active layer deepening, taliks, and retrogressive thaw slumps are some key examples of physical perturbations following permafrost change that have noted effects on local hydrogeochemical processes. Permafrost collapse and thaw features are able to quickly mobilize permafrost solutes such as particulate matter and dissolved inorganic solutes (Bowden et al. 2008; Lewis et al. 2012; Kokelj et al. 2013) to surface water flow paths (Turetsky et al. 2019) and lakes. Thermokarst is able to (1) reconnect surface water and surficial geology when materials are displaced (Kokelj and Jorgenson 2013); (2) create a transient impact on hydrological solute transport at smaller watershed scales (Larouche et al. 2015; Littlefair et al. 2017); (3) alter flow paths and transport nutrients and carbon originating from degrading permafrost and ground ice to aquatic systems (Abbott et al. 2015; Ma et al. 2019; Turetsky et al. 2019); (4) expose soil horizons that may have varying chemical compositions with depth (Lacelle et al. 2014); and (5) create mass wasting that in turn increases particulate, aged DOC, nutrients, and sediment transport to rivers, lakes, and streams within a watershed (Abbott et al. 2015; Walvoord and Striegl 2021). Active layer deepening allows permafrost organic C to become available for transport as DOC (Walvoord and Striegl 2021) can increase water storage and liberate frozen nutrients and mobile solutes (Lafrenière and Lamoureux 2019). Thaw slumps result in increased total suspended solids and specific conductivity, increasing the potential to alter the biological composition and food webs or affect rivers and lakes (Chin et al. 2016). Finally, taliks allow dispersive and advective solute migration to occur in supra and super permafrost zones (Johansson et al. 2015) and year-round subsurface mobilisation and delivery of dissolved C to inland waterways, changing the magnitude and seasonality of biogeochemistry and subsurface flow (Walvoord et al. 2019). However, such disturbances are often poorly characterised (Lake 2013), and failure to include these processes can result in underrepresentation of geochemical constituents in aquatic systems (Ma et al. 2019).

Flow paths (surface and subsurface) are another integral feature to consider in hydrogeochemical modelling of permafrost environments, yet our understanding and characterisation of subsurface hydrological flow paths is limited under these conditions (Walvoord and Striegl 2021). Hydrogeochemical predictions under climate change require the inclusion of subsurface processes (McKenzie et al. 2021) as hydrological transport pathways and connectivity change with climate warming and are expected to directly impact hydrochemistry (Frey and McClelland 2009; Vonk et al. 2015; Lamontagne-Hallé et al. 2018). The associated permafrost degradation can cause further changes to flow paths and associated dynamics (Ala-aho et al. 2018; Vonk et al. 2019; McKenzie et al. 2021). This subsequently creates new means for nutrients, carbon,

Table 2. Recent (2008 onwards) examples of hydrogeochemical models applied to permafrost environments.

Reference	Model	Model type	Model dimension	Region	Modelling aim	Missing processes
Yurova et al. (2008)	Mixed mire water and heat developed in the MATLAB module SIMULINK	Physically based, DOC concentration and fluxes in mire water using the convection-dispersion equation	• 1D vertical peat profile • 2D hydrological scheme (vertical discretization) for water movement	60 km northwest of Umea, Northern Sweden	Simulate DOC parameters and export for a small boreal mire	Permafrost
Bosson et al. (2013)	MIKE SHE	Physically based, groundwater flow and transport model	Three-dimensional	Forsmark catchment, ∼120 km north of Stockholm, Sweden	Simulate and quantify potential pathways and exchange of groundwater (deep and shallow) and solute transport between Quaternary deposits and bedrock using varying climate and permafrost conditions	Functionality for thermal modelling
Kicklighter et al. (2013)	Modified terrestrial ecosystem model	Process-based, biogeochemical model	N/A	Pan-Arctic watersheds	Estimate lateral transfer of DOC from land through river networks to the Arctic Ocean	Subsurface hydrological pathways
Frampton and Destouni (2015)	MarsFlo	Process-based, three-phase numerical, coupled cryotic and hydrogeological flow model, including particle tracking	2D rectangular domain	N/A—simulations represent a hypothetical cross-section in a catchment	Determine how subsurface flow, solute pathways, and travel times are impacted by permafrost thaw	
Lessels et al. (2015)	• Hydrologiska byrans vatten-blansavdelning rainfall-runoff model • DOC production component using modified ECOSSE soil carbon model algorithms	Process-based, parsimonious, coupled hydrological–biogeochemical model	N/A	Granger basin, within the Wolf Creek research basin, Yukon, Canada	Simulate stream discharge and daily DOC in a subarctic permafrost alpine catchment	Subsurface hydrological pathways
Grant et al. (2019)	*ecosys*	Process-based, terrestrial ecosystem biogeochemical model, including basic physical, chemical, and biological processes	Convective–diffusive solute transport based on thermal, hydraulic, gaseous, and aqueous conductivities in 2D (vertical and lateral) directions	∼6 km east of Barrow, Alaska, at the northern tip of Alaska's Arctic coastal plain	• Investigate the impacts of climate change on permafrost thaw • Investigate process rates in microbial and plant populations interacting with complex ecosystems, with soil water, gas, heat, and solute fluxes	Not focused on hydrological aspects
Bowring et al. (2020)	High-latitude-specific land surface component of ORCHIDEE MICT-LEAK (r5459)	Earth system model reproducing physical and biogeochemical processes	N/A	Lena River basin—bounded by the region 52–72°N and 102–142°E	Evaluate the river basin's output carbon fluxes and hydrological variables	No subsurface processes

Table 2. (*continued*).

Reference	Model	Model type	Model dimension	Region	Modelling aim	Missing processes
Yi et al. (2020)	• Remote-sensing-driven permafrost model • Coupled with a terrestrial carbon flux model	Process-based permafrost carbon model using mostly satellite remote-sensing data, coupled with a terrestrial carbon model	N/A	Model domain covered majority of Alaskan land area	Investigate how soil carbon emissions and the seasonal carbon cycle react to snow cover and climate regimes	Focused on snow (no rain-related processes)
Yi et al. (2021*a*)	MIN3P-HPC	Multicomponent reactive transport code to simulate primary thermo-hydro-chemical and mechanical processes	1D and 2D (1D hydromechanical coupling)	Meadowbank mine in the Kivialliq region (65°N, 96°W), in Nunavut, Canada	• Evaluate performance of thermal covers placed on waste rock piles • Assess thermo-hydrological–chemical processes of a sulfide-bearing waste rock pile with a thermal cover in a permafrost environment	• Not focused on groundwater or subsurface hydrological aspects • Not focused on natural environment
Yi et al. (2021*b*)	MIN3P-HPC	Multicomponent reactive transport code to simulate primary thermo-hydro-chemical and mechanical processes	• 1D (freeze–thaw capabilities to investigate sulfide mineral reactivity levels on a waste rock pile under warming climate conditions) • 2D (flow and reactive transport simulations)	Hypothetical pyrite-rich waste rock pile placed onto natural permafrost	Assess weathering of waste rock piles placed on permafrost	• Not focused on groundwater or subsurface hydrological aspects • Not focused on natural environment • Phase transformation between ice and water not explicitly included
Mohammed et al. (2021*a*)	Cryohydrogeological model built within FlexPDE	Physically based, numerical cryohydrogeo-logical model	• Limited to 2D mass and energy transport in the saturated subsurface • 2D topography-driven groundwater flow system • Surface energy balance first simulated using a 1D soil–vegetation–atmosphere transform model that informs the ground freeze–thaw conditions	• Wastewater lagoon facility in the NWT, Canada • Exact location not given for confidentiality reasons	Simulate solute transport in groundwater systems in permafrost environments	• Shallow subsurface flow • Subsurface flow, transport, and reaction property heterogeneities

Table 2. (*concluded*).

Reference	Model	Model type	Model dimension	Region	Modelling aim	Missing processes
Pongracz et al. (2021)	Lund–Potsdam–Jena general ecosystem simulator	Process-based, vegetation model, with improvements in simulating snow insulation and carbon pools	N/A	• Russian sites and pan-Arctic simulations • Northern circumpolar region above 60°N	• Simulate Arctic carbon-climate feedbacks • Simulate the insulating effects of snow, soil temperatures, and biogeochemistry	Not focused on subsurface hydrological aspects or groundwater

Note: Table includes the study reference, model(s) used in the simulation, model type, aim of the simulation, model dimension(s), region(s) simulated, and notable processes missing from the study when considering future hydrogeochemical permafrost modelling. An N/A under the "model dimension" column indicates that the study did not explicitly state the modelling dimension. 1D, one-dimensional; 2D, two-dimensional.

and dissolved constituents to be transported (McKenzie et al. 2021). Changes in groundwater dynamics and flow paths have been shown to impact geochemistry by (1) creating links between organic matter mobilisation and flow paths (Striegl et al. 2005; Walvoord and Striegl 2007, 2021; Lafrenière and Lamoureux 2019); (2) enhancing conservative solute transport while increasing solute reactions and sorption to the unfrozen materials in the ground (Mohammed et al. 2021*a*); (3) increasing permafrost soil vulnerability to soluble C and N release (Wickland et al. 2018), allowing perennial suprapermafrost flow and C transport (Walvoord et al. 2019); and (4) increasing calcium, magnesium, sodium, sulfate, and phosphorus fluxes through flow path deepening (Toohey et al. 2016). Further, if solute-rich deep soils are hydrologically connected, thermal perturbations can transport seasonally large inorganic solute loads (Lafrenière and Lamoureux 2019). When included in modelling, subsurface processes are often constrained to the vertical dimension with low vertical spatial resolution. Furthermore, Earth system models do not typically include groundwater and lateral chemical export (McKenzie et al. 2021).

Together, transfers of water, heat, and solutes strongly influence the maximum extent and distribution of solute mass within a system (Mohammed et al. 2021*a*). These processes are often interrelated. Their incorporation into models would help avoid under-representing the rate and magnitude of environmental changes (McKenzie et al. 2021). Failure to incorporate these processes can result in poor model performance for simulating hydrogeochemical processes. For example, the exclusion of deep flow mechanisms in hydrological model formulation can result in poor model flow in periods of low flow (Yurova et al. 2008) and failure to include lateral hydrological C flux (McGuire et al. 2018) can result in an underestimation of dissolved C transport response to inland thaw (Gao et al. 2021). Additionally, many Earth system models ignore permafrost–climate–carbon feedbacks because the associated land models do not incorporate vertically resolved C soil dynamics (McGuire et al. 2018). The critical processes to consider in future hydrogeochemical modelling of permafrost environments are summarised in Fig. 1.

The simulation of these key processes requires the consideration of several parameters and variables when assessing model suitability. Ultimately, model choice will depend on the study objectives, which will dictate relevant physical processes to be included in a conceptual model, and the scale of study (Lamontagne-Hallé et al. 2020). In the following subsections, we discuss some of the major modelling considerations proposed by Lamontagne-Hallé et al. (2020), in addition to critical parameters and variables, in the context of hydrogeochemical modelling in permafrost environments. These considerations are summarised into two schematic diagrams depicting the critical processes, parameters, and variables (Fig. 1) and key considerations for computational resources and limits (Fig. 2) for future hydrogeochemical modelling efforts in permafrost environments.

5.2. Parameters and variables

Several model parameters are often needed to adequately constrain hydrogeochemistry models for permafrost environments and ensure that relevant processes are properly represented (Fig. 1). These parameters include soil texture, moisture, and parent material (Jacobson et al. 2002; Moquin and Wrona 2015; Wickland et al. 2018; Vonk et al. 2019; Elshamy et al. 2020; Tank et al. 2020); landcover and vegetation (Frey and McClelland 2009; Yu et al. 2010; Ma et al. 2019; Treat et al. 2019); topography, relief, slope, aspect, and geomorphology (Kicklighter et al. 2013; Painter et al. 2013; Jasechko et al. 2016; Kutscher et al. 2017; Ma et al. 2019; Vonk et al. 2019; Bowring et al. 2020); and processes governing the division of water and its transit and residence times (Douglas et al. 2013; Kicklighter et al. 2013; Kokelj et al. 2013; Olefeldt et al. 2016; Cochand et al. 2019; Vonk et al. 2019; Tank et al. 2020; Mohammed et al. 2021*a*, 2021*b*; Pongracz et al. 2021). Table 3 includes individual parameters of permafrost environments and their importance for future hydrogeochemical modelling. The interplay of the different parameters noted in Table 3 can influence many important hydrogeochemical processes in permafrost regions. Table 4 illustrates some noted combinations of model parameters and the processes they help elucidate. The feedbacks between hydrology, permafrost state, and geomorphology (e.g., thaw slumps) suggest that several of these parameters often require spatial and temporal adjustment to capture heterogeneity and seasonality within the model structure.

In particular, the spatial continuity of permafrost is rarely incorporated in permafrost biogeochemical modelling (Fabre et al. 2017). Yet, permafrost coverage has been noted as a primary control of regional hydrology (Ala-aho et al. 2018).

Fig. 1. Simplified conceptual schematic diagram highlighting the critical processes, parameters, and variables to consider for future hydrogeochemical modelling efforts in permafrost environments. The critical processes are numbered 1–23 in the schematic and listed under their associated panel (i.e., "Hydrological", "Thermal", "Physical", or "Chemical"). Critical parameters and variables are listed underneath the schematic. The critical processes are discussed in Section 5.1, and the parameter and variable data to elucidate crucial processes are discussed in Section 5.2 and in Tables 3 and 4.

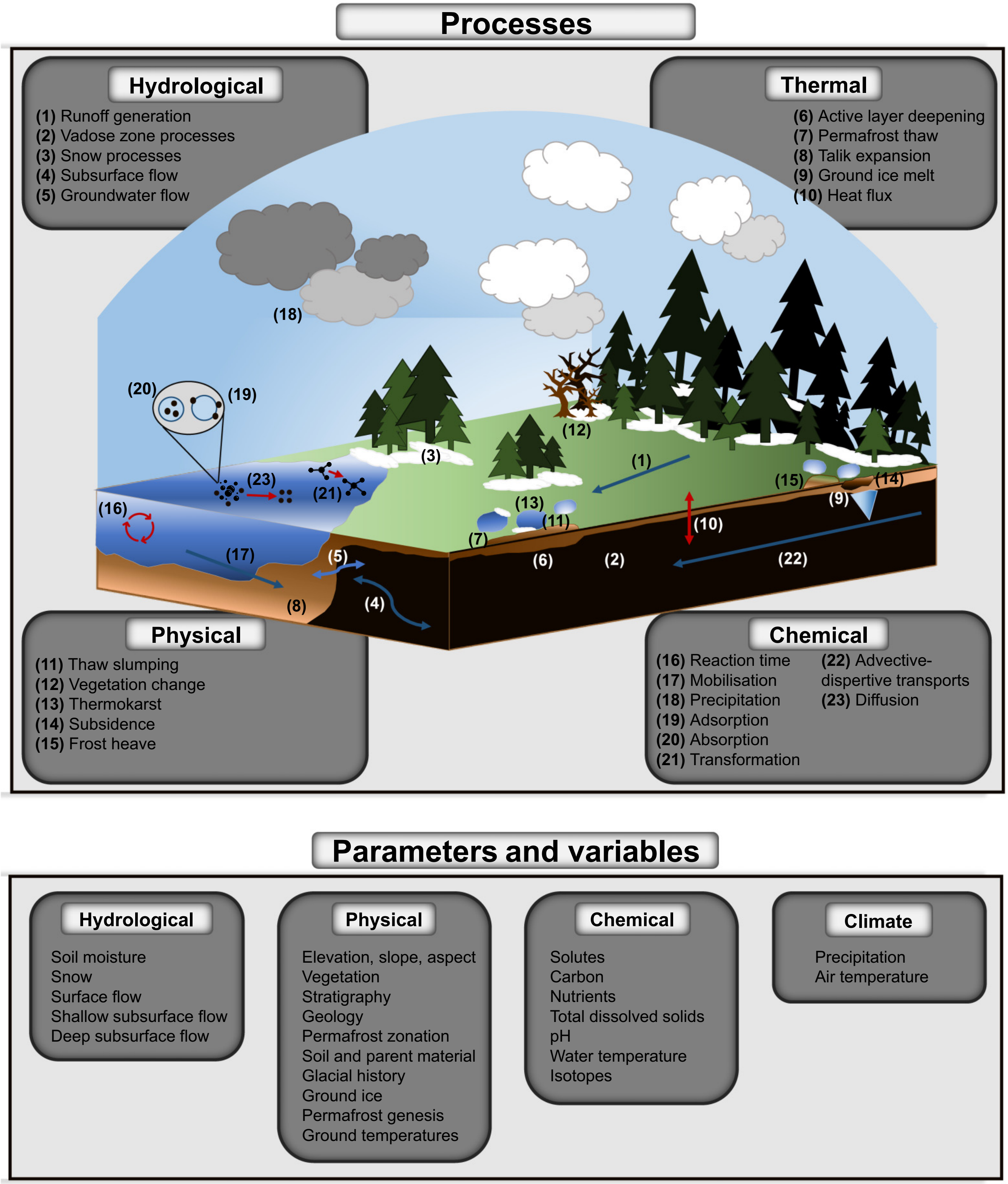
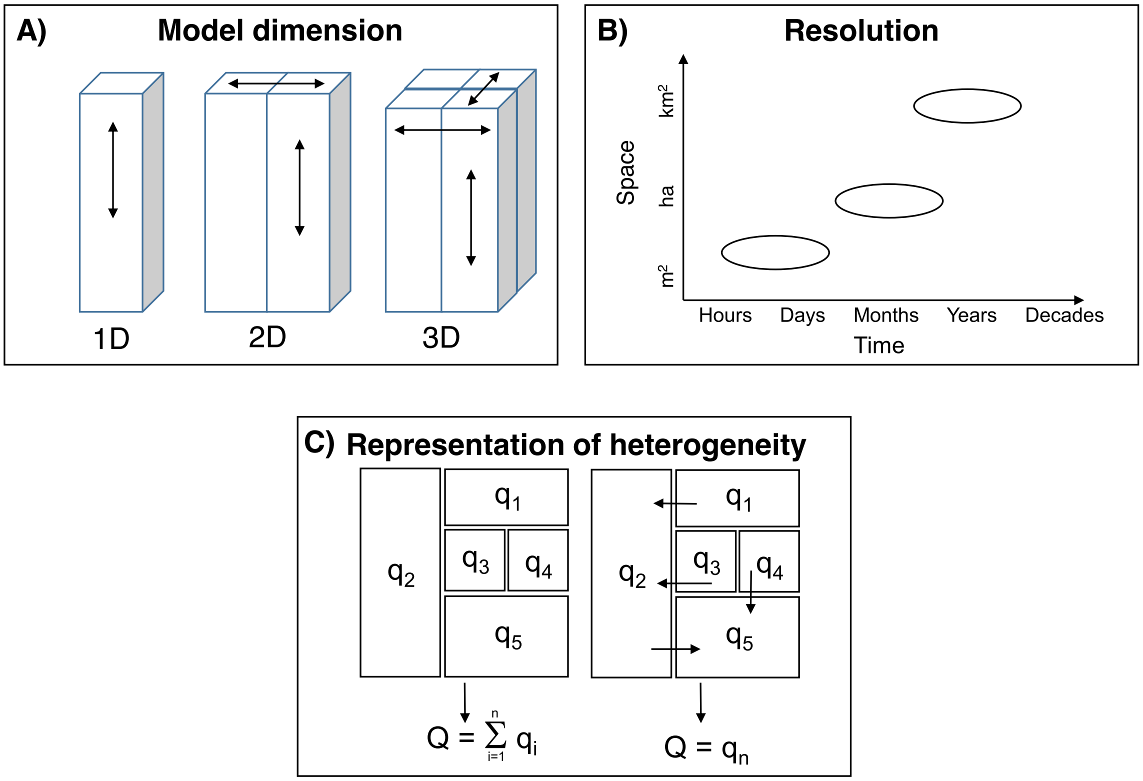


Fig. 2. Key considerations for computational resources and limits for future hydrogeochemical modelling efforts in permafrost environments. (A) Illustration of the three types of model dimensionality available for simulations. (B) Illustration of the trade-offs and considerations when choosing model resolution in both space and time. Spatially, resolutions can range from small (m^2) to large (km^2), while temporal resolution can range from hours to decades. The ovals represent the increasing computing power constraints resulting from higher temporal and spatial resolutions. (C) Representation of heterogeneity when upscaling mass and energy fluxes from the subgrid to grid scale. Heterogeneity can either be calculated as the sum of all the subgrid fluxes (left) or account for subgrid connectivity (right). Sections 5.3, 5.4, 5.5, and 5.6 of the paper describe many aspects of model structure, computational resources, and limits.



Permafrost zonation can impact hydrological components, including flow paths, residence times in water, and permeability (Vonk et al. 2019) or act as an effective barrier to contaminant migration (Mohammed et al. 2021*a*). In turn, this can influence geochemical activities in these environments (e.g., the composition, age, and quantity of mobilised C, affecting its fate (Vonk et al. 2019)). Discontinuous to sporadic permafrost regions are characterised by more advanced thaw stages (Walvoord and Striegl 2021) and are the most susceptible to near-term thaw (Walvoord and Kurylyk 2016). Further, discontinuous permafrost environments include a larger variation in permafrost depths, which impacts hydrological connectivity if permafrost thaws and increases the potential for water and solute exchange in areas above and below permafrost (Vonk et al. 2019). In contrast, the continuous permafrost zone is associated with the least advanced thaw stages (Walvoord and Striegl 2021). Overall, regions vulnerable to complete permafrost loss (more than 4 m) are the most hydrogeologically relevant as they create subsurface connectivity and therefore require site-specific considerations and parameterization to understand the impacts of this loss (Walvoord and Striegl 2021).

5.3. Model dimension

The choice of model dimension will determine how processes can be represented (Fig. 2). Freeze–thaw processes (Walvoord and Kurylyk 2016), heat flux (Jorgenson et al. 2010), and hydrological flow (Painter et al. 2013) are multidimensional in permafrost environments and therefore crucial to consider when choosing a model dimension for simulating the response of hydrogeochemical processes to climate change. Processes with a lateral component influence soil freezing and heat flux and are particularly important to consider when investigating permafrost in isolated patches and discontinuous permafrost zones (Kurylyk et al. 2016; Sjöberg et al. 2016; Walvoord and Kurylyk 2016; Bui et al. 2020). Two-dimensional (2D) and 3D models can potentially resolve and capture thermal processes for complex Arctic landscapes more accurately (Yi et al. 2014) and in turn incorporate the critical multi-dimensional processes occurring in permafrost environments. For example, riparian zones are characterised by high microbial and biogeochemical cycling and high hydrological connectivity (Bonnaventure et al. 2017). Water bodies and wetlands located adjacent to permafrost impact lateral thaw (Devoie et al. 2021) and groundwater flow, influencing heat advection in multiple directions around

Table 3. Parameters of permafrost environments important to consider in hydrogeochemical modelling efforts.

Parameters	Importance for hydrogeochemical modelling	Reference(s)
Soil texture, soil moisture, and parent material	Help simulate permafrost characteristics	Elshamy et al. (2020)
	Dictate leaching yield	Wickland et al. (2018)
	Dictate amount of mineral sorption of organic matter	Vonk et al. (2019)
	Dictate major cations and anions present in soil column	Moquin and Wrona (2015)
	Influence biogeochemical processing, permeability, and composition of thawed permafrost and active layer	Tank et al. (2020)
	Impact water chemistry	Jacobson et al. (2002)
	Accumulation and degradation of soil carbon	Schuur et al. (2009)
	Source of DOC and total dissolved nitrogen	Lessels et al. (2015); Wickland et al. (2018)
	Simulation of how soil hydraulic properties influence hydrochemical processes and the persistence and fate of solutes	Lawrence et al. (2011); Swenson et al. (2012); Mohammed et al. (2021*a*)
Transit and residence times	Elucidate spatial extent and impact of hydrogeochemical responses	Tank et al. (2020)
Land cover and vegetation	Aquatic DOC primarily originates from terrestrial plants and soils	Ma et al. (2019)
	Peat and peatlands have notable hydraulic conductivity properties and can store large organic carbon and nitrogen stocks	Yu et al. (2010); Treat et al. (2019)
	Peat can have enhanced DOC fluxes following deep thaw and increased flow	Frey and McClelland (2009)
Topography, relief, slope, and aspect	Regulate thaw response	Vonk et al. (2019)
	Impact long-term accumulation of ground ice and organic matter	Vonk et al. (2019)
	DOC export	Ma et al. (2019)
	DOC concentrations	Bowring et al. (2020)
	Provide means for lateral transport of particulate and dissolved material	Vonk et al. (2019)
	Influence hydraulic gradients, resulting in increased water fluxes, decreased transit times, and increased ability for lateral carbon movement	Vonk et al. (2019)
	Controls the mobilization of particulate and dissolved constituents	Vonk et al. (2015)
	Predicts water infiltration depth, concentration, and DOC age	Jasechko et al. (2016); Kutscher et al. (2017)
	Snowmelt and soil thaw occur on south-facing slopes before north-facing slopes, impacting hydrological and biogeochemical activities	Kicklighter et al. (2013)
Ground ice	Influences chemical constituent contents	Vonk et al. (2019); Mohammed et al. (2021*a*)
	Ice-rich permafrost thaw can mobilize particulate constituents; ice-poor permafrost can release dissolved constituents	Kokelj et al. (2013); Olefeldt et al. (2016)
Snow	Snowmelt runoff quickly transports nutrient exports to surface	Douglas et al. (2013)
	Model performance restricted by snow complexity representation in model	Pongracz et al. (2021)
	Local-scale snow dynamics impact carbon fluxes through changes in soil thermal conditions and vegetation habitat	Pongracz et al. (2021)
Surface and subsurface runoff	Talik presence impacts groundwater flow dynamics, subsequently influencing spatial distribution of solutes	Mohammed et al. (2021*a*)
	In-stream carbon dynamics influence DOC degradation and yearly loss	Kicklighter et al. (2013)

Note: DOC, dissolved organic carbon.

permafrost (Kurylyk et al. 2016; Devoie et al. 2021). Difficulties in deploying 3D simulations include issues employing models over larger domains (Yi et al. 2014) and large computational demands associated with the required smaller time steps needed to predict permafrost thaw and climate change impacts across three dimensions (Lamontagne-Hallé et al. 2020). These difficulties have forced many to pursue one-dimensional (1D) or 2D vertical plane, permafrost modelling efforts. However, 1D modelling approaches may be less suitable for simulating many hydrogeochemical processes associated with permafrost change. In addition to the limitations associated with the multidimensional processes noted above, a 1D model is limited in temporal scale because multi-year changes often involve multidimensional changes,

Table 4. Combinations of model parameters and the relevant processes they help elucidate related to hydrogeochemical modelling in permafrost regions.

Model parameters and variables	Elucidated processes	Reference
Surface water runoff, groundwater flow, snow, vegetation, and topography	Thermal regime of permafrost	Jorgenson et al. (2010)
Temperature, slope, permafrost extent, parent material, and permafrost material age	Dissolved matter's water infiltration fluxes and transformations	Bowring et al. (2020)
Ice content, relief, permafrost extent, and parent material	Northern landscape change	Tank et al. (2020)
Glacial history, ice content, and parent material	Water chemistry	Abbott et al. (2015)
Ice content, soil, topography, and permafrost extent	Potential, rate, and biogeochemical and hydrological thaw impacts	Vonk et al. (2015)
Temperature, precipitation, and atmospheric CO_2	DOC discharge	Bowring et al. (2020)

thus making 1D modelling approaches more appropriate for seasonal unilateral freeze–thaw processes instead of multi-year or decadal processes (Walvoord and Kurylyk 2016; Bui et al. 2020). Therefore, 1D and 2D models may adequately simulate cold-region subsurface processes given the right approach (Jan et al. 2018) that incorporates targeted simplifications or assumptions of the investigated system (Riseborough et al. 2008), while a 2D or 3D environment would be better suited to simulate many parameters and the multi-dimensional characteristics of permafrost regions, but they may be more limited in the spatial extent and resolution due to computational costs.

5.4. Representation of landscape heterogeneity

Related to model dimensionality is the ability of the model to represent landscape heterogeneity. Permafrost regions are characterised by notable landscape heterogeneity (French 2017) that creates heterogeneous permafrost thaw and associated subsurface connectivity (Walvoord and Kurylyk 2016; Rey et al. 2019) with commensurate freshwater system impacts (Walvoord and Kurylyk 2016; McKenzie et al. 2021). Permafrost and hydrological heterogeneities result in varying biogeochemical transport and fate across small scales (Jones et al. 2020). High sub-grid manifestation of temporal and spatial heterogeneities of processes creates variation in patterns of soil properties, vegetation (Endalamaw et al. 2017), taliks and thermokarst, soil subsidence, runoff (Andresen et al. 2020), and heat dynamics (Yi et al. 2014; Andresen et al. 2020). Large-scale models must include upscaling of these generally local- or site-scale processes (Andresen et al. 2020) (Fig. 2). Geochemical heterogeneity in permafrost regions includes (1) the spatial variability of N (Harden et al. 2012) and C (Hugelius et al. 2013); (2) variable DOC and TDN release following permafrost thaw (Wickland et al. 2018); (3) seasonally variable biogeochemical signatures in northern rivers (Douglas et al. 2013); and (4) aquatic C response to climate change in the discontinuous permafrost zone (Tank et al. 2020). Likewise, biogeochemical response to climate change is regionally variable, related to variability in thaw drivers (Tank et al. 2020), resulting in different chemical concentrations in aquatic systems (Harms et al. 2014; Mann et al. 2015) following permafrost degradation.

Substantial spatial data are required to quantify the heterogeneity of hydrological factors across the circumpolar north to avoid biases at finer scales (Shogren et al. 2019; Tank et al. 2020). However, the lack of such detailed data often leads to many studies smoothing the representation of heterogeneity in hydrological models (Walvoord et al. 2019). Knowledge of spatial and temporal variability and reasons for change in terrestrial permafrost landscapes can only be elucidated through advancements in the representation of biogeochemical heterogeneity in models (Andresen et al. 2020). This may require 3D models (Painter et al. 2016), with the understanding that, as models are real-world simplifications, it is unrealistic and not always necessary to include all heterogeneous processes in a model. For example, sub-grid parameterization methods have been successfully incorporated into modelling to represent heterogeneous soil thermal and hydraulic parameters (Endalamaw et al. 2017). Therefore, the critical aspect of future hydrogeochemical modelling will be determining which processes should be included and which can be simplified (Gao et al. 2021).

5.5. Model scale and spatiotemporal resolution

Modelling scale and spatiotemporal resolution are other important considerations related to the heterogeneous nature of permafrost environments. The temporal and spatial scale chosen for the model will influence the parameters needed and the resulting model performance because the impact of a process on local hydrology depends on both scale and the environmental setting (Lamontagne-Hallé et al. 2020) (Fig. 2). Geochemistry can be scale-dependent, yet biogeochemical signals at various temporal and spatial scales are poorly understood in diverse catchments (Shatilla and Carey 2019). Geochemical temporal variation exists in reaction rates (Tank et al. 2020), DOC/TDN ratios (Douglas et al. 2013), and ionic dissolution (Moquin and Wrona 2015). Temporal variation exists for permafrost response to climate change, with physical and thermal perturbations varying in both frequency and recovery time. Physical disturbances can occur over long durations, ranging from years to decades (Malone et al. 2013; Lamoureux et al. 2014; Lamhonwah et al. 2017), with predictions suggesting an increase in their temporal frequency (Smith et al. 2022) and the observational scale significant in determining duration

(Lafrenière and Lamoureux 2019). For example, a marked increase in retrogressive thaw slumps has been noted in recent decades (Lewkowicz and Way 2019; Ward Jones et al. 2019). Flow paths leading to subarctic rivers vary throughout the year requiring longer-term modelling scales that incorporate the multiple flow regimes that exist during the annual cycle (Douglas et al. 2013). The dynamic nature of permafrost regions necessitates longer temporal model configurations as permafrost has a heterogeneous spatio-temporal response to climate change that evolves over time (e.g., Zhang 2013). However, limitations exist for longer time scales as coarser time steps may result in modelling inaccuracies (Anderson et al. 2015). For example, daily time-step models have resulted in more accurate predictions, with monthly time steps typically impeding understanding of water pathways and freshet (Fabre et al. 2017). Model time scales should also not be so long as to mute finer-resolution components on intra-yearly events. For example, large yearly nutrient fluxes can be associated with relatively short-lived flow events and phenomena (Douglas et al. 2013).

Spatially, differences in geographic extent, landscapes, and hydrological conditions will (1) result in variability between the form, pathway, and magnitude of constituent release from flow pathways (Vonk et al. 2015); (2) impact how DOC flux changes with climate change and mixed DOM signals (Shatilla and Carey 2019); and (3) result in differing reaction rates (Tank et al. 2020). Field-based studies have shown that scaling solute behaviour to fit various landscapes can be effective (Shogren et al. 2019). However, most permafrost models often do not downscale for hydrological processes (Fabre et al. 2017), resulting in difficulty reproducing small-scale processes. For example, intermediate landscape scales ranging from 3 to 30 km^2 are important regulators of Arctic C and nutrient sinks and sources (Shogren et al. 2019).

5.6. Additional considerations and limitations

Modelling is a means to investigate questions regarding hydrogeochemistry where a lack of empirical information exists (Lessels et al. 2015). The primary limitation noted in previous hydrogeochemistry-related modelling in permafrost environments is the lack of relevant field and experimental data (e.g., Kicklighter et al. 2013; Lake 2013; Lessels et al. 2015; Tetzlaff et al. 2015; Angeler and Allen 2016; Walvoord and Kurylyk 2016; Li Yung Lung et al. 2018; Treat et al. 2019; Vonk et al. 2019; Andresen et al. 2020; Chaudhary et al. 2020; Elshamy et al. 2020; Hugelius et al. 2020; Tank et al. 2020; Gao et al. 2021; McKenzie et al. 2021; Mohammed et al. 2021*a*; Walvoord and Striegl 2021) and the fulfillment of associated research needs (Tetzlaff et al. 2015; McKenzie et al. 2021; Mohammed et al. 2021*a*), particularly in areas responding quickly to climatic changes (Tetzlaff et al. 2015). The lack of relevant data can result in many modelling deficiencies, including poor definition of seasonally variable parameters during freeze and thaw. Therefore, future biogeochemical permafrost modelling efforts should ensure that model complexity is appropriate for the available data (Beven and Freer 2001) and to accept that not all field observations can be simulated (Konikow 2011). Computational limitations may challenge the implementation of 3D hydrogeochemical models (Lamontagne-Hallé et al. 2020) and 2D models at increased resolutions (Walvoord and Kurylyk 2016) or the incorporation of the large spatial heterogeneity of permafrost environments (Gao et al. 2021). These limitations have resulted in the over-simplification of processes included in large-scale Earth system models, specifically those used to simulate dynamic water and carbon changes in thawing permafrost environments (Walvoord and Striegl 2021). The complexity of some geochemical components (e.g., DOC) can also result in hesitancy to incorporate them into models (Ma et al. 2019).

An important first step in hydrogeochemical modelling of permafrost environments is to identify the relevant processes for a specific landscape instead of attempting to include all types of processes and mechanisms in tools that are already extremely complex (Lamontagne-Hallé et al. 2020). Increasing the complexity of a model may decrease its accuracy as more parameters are required to be calibrated and estimated, leading to increased uncertainty (Voss 2011; Lamontagne-Hallé et al. 2020). Before creating a sophisticated hydrogeochemical model for permafrost regions, it is essential to evaluate existing model performance and identify limitations (e.g., Domine et al. 2019). Further, the critical processes, inputs and outputs, and structure need to be assessed (Figs. 1 and 2) during model development, as excessive complexity can strongly affect computational efficiency (Lamontagne-Hallé et al. 2020). Model choice will also be important as simulations must have the ability to include the required processes and parameters (Figs. 1 and 2). Specific models used in previous work that have either exhibited or appear to have the potential to simulate hydrogeochemistry in permafrost environments are summarized in Table 5.

The final element to consider for future hydrogeochemical permafrost modelling efforts is which region(s) should be simulated. Zones of high aquatic and biogeochemical importance, such as channel beds in riparian zones (Bonnaventure et al. 2017), may be useful starting points for a modelling environment. Modelling has been identified as a priority for regions within the discontinuous–continuous permafrost transition zone (Vonk et al. 2015; Walvoord and Striegl 2021) because flow processes change from a more shallow warm season to deeper year-round processes, a change predicted to influence the lateral transport of hydrological C (Walvoord and Striegl 2021). Additionally, environments susceptible to thermokarst development are another region of interest because of the carbon liberation associated with these thawing processes (Vonk et al. 2015). However, modelling the hydrogeochemical response to permafrost change in the discontinuous permafrost zone can be challenging because of transient surface and subsurface flow paths and variable fluxes and residence times in the transition zone between continuous and discontinuous permafrost (Walvoord and Striegl 2021). To help narrow the field of study, the Canadian Water Resource Vulnerability Index to Permafrost Thaw (Spence et al. 2020), for example, could be used to assess specific areas within the discontinuous–continuous permafrost transition zone that are particularly vulnerable to thaw.

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Table 5. Models that have either exhibited or been suggested to have potential for future hydrogeochemical simulations in permafrost environments.

Model(s)	Type	Relevant abilities	Reference suggesting model usage
PFLOTRAN-ice	Reactive flow and transport model	Heat transfer, solute transport, multiphase flow routines	Bui et al. (2020); Mohammed et al. (2021*a*)
Cryohydrogeolical numerical simulator in OpenFoam	Water and energy transfer model	Heat transfer, solute transport, multiphase flow routines	Mohammed et al. 2021*a*)
Hydrologiska byrans vattenbalansavdelning (HBV) model coupled with thermal models	Hydrological model coupled with thermal models or biogeochemical models	Estimate nutrient loads	Lessels et al. (2015); Bui et al. (2020)
SWAT, including hydrological functions of permafrost	Hydro-agro-climatological model	Simulate biogeochemical flows in permafrost soils	Fabre et al. (2017)
Ecological model for applied geophysics	Surface hydrological model	Simulate horizontal water flow, geochemical processes, and biochemical degradation processes of dissolved organic pollutants	Bui et al. (2020)
Cryohydrogeological model built within FlexPDE	Cryohydrogeological model	Greater model applicability throughout a range of permafrost environments	Mohammed et al. (2021*a*)
SUTRA-ICE model with two-dimensional and three-dimensional options	Cryohydrogeological model	Simulate both saturated and unsaturated groundwater flow and solute and energy transport	Bui et al. (2020)

Note: The models included in this table have not necessarily been employed for this use as of yet.

6. Recommendations for future hydrogeochemical modelling efforts in permafrost environments

We reviewed the recent literature on hydrogeochemical modelling in permafrost areas and related science fields. The results were used to identify research gaps and lessons learned from previous modelling attempts. Overall, our review highlighted that most studies incorporating a geochemical modelling component focus predominantly on carbon dynamics and/or do not include subsurface hydrological pathways. Our work aims to inform future research in this field, which has become critical with the increasing threat of climate change accelerating permafrost thaw and the release of DOC and other chemical constituents. We have summarized the key takeaway messages into eight recommendations for future efforts aimed at incorporating hydrogeochemical modelling in permafrost environments:

1) Improving biogeochemical models for permafrost regions requires strengthening synergies between the biogeochemical and cryohydrogeological communities, potentially using shared modelling frameworks that can provide mutual benefit, reduce oversimplifications, and eliminate duplication of work.
2) Future models should consider heat transfer processes, heat fluxes and freeze-thaw regimes, impacts on biogeochemical processes and rates (e.g., seasonality, permafrost disturbance, and snow–soil–vegetation feedbacks), permafrost zonation, and subsurface flow paths (Fig. 1).
3) The following model parameters should be considered for inclusion in simulations: soil texture, moisture content and parent material, landcover and vegetation, topography, relief, slope, aspect and geomorphology, and parameters governing the division of water and its transit and residence times (Fig. 1).
4) The spatial heterogeneity of hydrology, geochemistry, and permafrost landscapes should be represented in large-scale models with as much detail as possible within the limits of computational costs (Fig. 2).
5) Temporal variation needs to be considered. Longer timescales are recommended while ensuring the temporal scale does not mute finer-resolution components or intra-yearly events (Fig. 2).
6) Modelling efforts should ensure that model complexity is appropriate for the study objectives and available data while understanding that not all variables and processes can or need to be simulated.
7) 2D and 3D models can capture thermal processes for complex permafrost environments by incorporating the associated critical multi-dimensional processes, while 1D models can be employed where computational demands prohibit the use of 2D or 3D modelling, and/or with the aim of targeting simplifications or assumptions of the investigated system.
8) Zones of high aquatic and biogeochemical importance (e.g., the riparian zone) that are particularly vulnerable to thaw within the discontinuous–continuous permafrost transition zone are suggested as initial sites for first modelling attempts.

7. Conclusion

Our review of the recent literature relevant to hydrogeochemical modelling in permafrost environments resulted in a discussion of key processes to consider when assessing the feasibility and potential for modelling hydrogeochemistry in permafrost environments, including heat transfer and associated freeze–thaw regimes, biogeochemical cycles and rates, and surface and subsurface flow pathways. Following this, we discussed additional considerations (e.g., model dimension, scale, heterogeneity, permafrost zonation, and boundary conditions) and key model parameters needed at different spatio-temporal scales. Finally, we provided a simplified conceptual schematic (Fig. 1) that includes the processes mentioned above and parameter considerations and a schematic of considerations and limits (Fig. 2) for future modelling of hydrogeochemistry in permafrost environments. We conclude that incorporating biogeochemistry in permafrost modelling is a difficult problem due to the highly heterogeneous nature of permafrost regions and the interplay between physical, climate, hydrological, and biogeochemical processes. Substantial progress has been made over the last decades, but the lack of relevant field data coupled with the compromise between computational limitations and accurate representation of processes and spatiotemporal scales remain major obstacles. We argue that improving biogeochemical models for permafrost regions will require strengthening coordination between the biogeochemical and cryohydrogeological communities, potentially adopting shared modelling frameworks that can provide mutual benefit, reduce oversimplifications, and eliminate duplication of work.

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