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PRIMER

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Guidelines for cold-regions groundwater numerical modeling

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Abstract
The impacts of ongoing climate warming on cold-regions hydrogeology and groundwater resources have created a need to develop groundwater models adapted to these environments. Although permafrost is considered relatively impermeable to groundwater flow, permafrost thaw may result in potential increases in surface water infiltration, groundwater recharge, and hydrogeologic connectivity that can impact northern water resources. To account for these feedbacks, groundwater models that include the dynamic effects of freezing and thawing on ground properties and thermal regimes have been recently developed. However, these models are more complex than traditional hydrogeology numerical models due to the inclusion of nonlinear freeze–thaw processes and complex thermal boundary conditions. As such, their use to date has been limited to a small community of modeling experts. This article aims to provide guidelines and tips on cold-regions groundwater modeling for those with previous modeling experience.

This article is categorized under:
- Engineering Water > Methods
- Science of Water > Hydrological Processes

KEYWORDS
cold regions hydrology, cryohydrogeology, groundwater modeling, hydrogeology, permafrost

1 | INTRODUCTION

High-latitude terrestrial environments are warming at twice the global rate (Meredith et al., 2020), resulting in pronounced decreases in the extent of permafrost (i.e., ground that remains below 0°C for at least 2 consecutive years, Romanovsky, Smith, & Christiansen, 2010; Walsh et al., 2005). Climate models project that between 29% and 90% of the area currently underlain by permafrost will become permafrost-free by 2,300, with most of the loss occurring before 2,100 (McGuire et al., 2018). Permafrost thaw results in cascading environmental impacts, including land subsidence, and slope instability, that are concerning for northern communities and industry (Teufel & Sushama, 2019). Furthermore, because the release of sequestered carbon from permafrost is transitioning many cold regions into a global source of carbon (Campbell, 2019), permafrost thaw can result in a positive climate change feedback that accelerates future warming (Schuur et al., 2015).

Permafrost is often considered impermeable because ice in pores will impede or block groundwater flow (Williams & Smith, 1989). Hence, in permafrost regions, groundwater flow can occur in the seasonally-thawed active layer above permafrost, in sub-permafrost aquifers below the permafrost, and in perennially unfrozen zones called taliks (Woo, 2012; Figure 1a,b). When the pore ice melts, hydraulic conductivity may increase by several orders of magnitude, thereby increasing both the velocity of groundwater flow through the now unfrozen ground and increasing the infiltration rate of surface water into the ground (Kurylyk & Watanabe, 2013). These dynamic groundwater flow systems can sustain perennial flow networks between aquifers and surface water bodies through unfrozen pathways (Devoie, Craig, Connon, & Quinton, 2019; Jepsen, Voss, Walvoord, Minsley, & Rover, 2013; Walvoord & Kurylyk, 2016) (Figure 1c,d). However, the overall effect of permafrost thaw on groundwater flow systems, and more particularly on groundwater–surface water interactions, remains unknown, with studies suggesting that these interactions can be highly variable and dependent on the physical setting (Lemieux et al., 2020; McKenzie et al., 2020; Walvoord & Kurylyk, 2016). For example, the impact of permafrost thaw on northern groundwater resources is mixed—some communities will suffer from a loss of surface water availability due to permafrost thaw (e.g., Smith, Sheng, MacDonald, & Hinzman, 2005; White, Gerlach, Loring, Tidwell, & Chambers, 2007), while others may benefit as newly formed aquifers created by permafrost thaw can provide critical drinking water resources (Lemieux et al., 2016). Groundwater processes in permafrost environments are also of great importance for northern infrastructure (McKenzie et al., 2020), as heat advection may accelerate thawing and environmental changes. As examples,

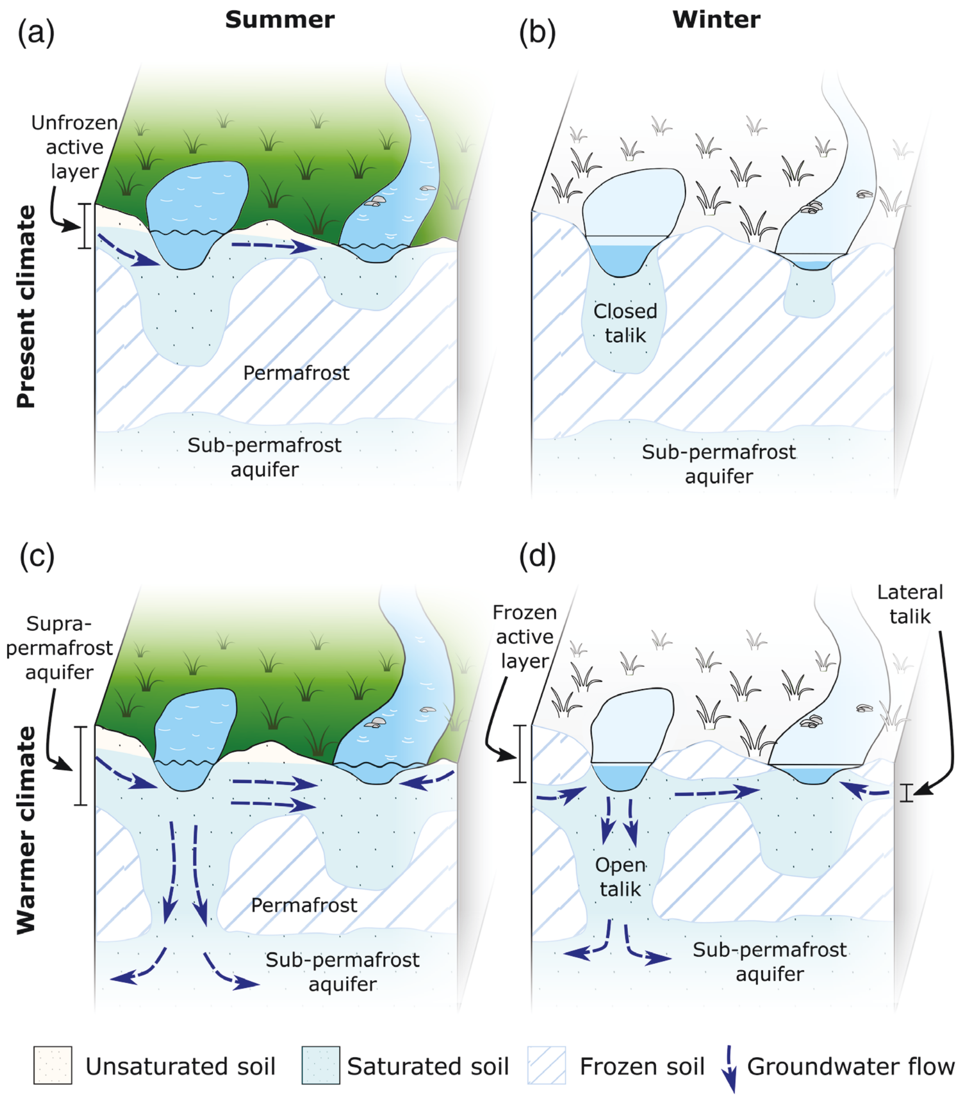


FIGURE 1 Conceptual hydrogeologic permafrost systems under the present climate conditions for (a) summer and (b) winter, and its potential changes in a warmer climate for (c) summer and (d) winter

cryohydrogeology is important for thawing under road embankments (Chen, Fortier, McKenzie, & Sliger, 2020) and the formation of aufeis (or icing) (Chesnokova, Baraër & Bouchard, 2020; Ensom et al., 2020). Permafrost thaw and groundwater flow also affects mining development in northern regions, leading potentially to increased dewatering and contaminant transport in mine tailings storage systems (Elberling, 2004; Journeaux Associates, 2012). The lateral transport of previously sequestered carbon through horizontal groundwater pathways is also of considerable interest (Neilson et al., 2018; Vonk, Tank, & Walvoord, 2019) given that it is neglected or handled as a residual in most large-scale biogeochemical models (e.g., McGuire et al., 2018).

Due to the lack of field-based knowledge and predictions of hydrological trends in cold regions, several multi-dimensional numerical models have been developed over the last decade to investigate the processes that control groundwater systems in cold regions (e.g., Bense, Kooi, Ferguson, & Read, 2012; Endrizzi, Gruber, Dall'Amico, & Rigon, 2014; McKenzie, Voss, & Siegel, 2007). These cold-regions groundwater models, also called cryohydrogeologic models, are usually developed by enhancing an existing three-dimensional coupled groundwater flow and energy transport model through the inclusion of dynamic freezing and thawing and the effects on the soil's energy balance and hydraulic and thermal properties. Most of the studies that use these models have considered archetypical cold hydrogeological environments, with the objective of developing a conceptual understanding of these complex settings and how they respond to warming (e.g., Bense et al., 2012; Frampton, Painter, & Destouni, 2013). Research efforts to date have highlighted the importance of heat advection through groundwater flow as a possible contributor to permafrost degradation in certain settings (Dagenais, Molson, Lemieux, Fortier, & Therrien, 2020; McKenzie & Voss, 2013; Shojae Ghias, Therrien, Molson, & Lemieux, 2018; Sjöberg et al., 2016), elucidated the formation and hydrogeological impact of lateral and vertical taliks (Jafarov et al., 2018; Lamontagne-Hallé, McKenzie, Kurylyk, & Zipper, 2018; Rowland, Travis, & Wilson, 2011; Wellman, Voss, & Walvoord, 2013), illustrated the current and future patterns of groundwater discharge to streams (Evans, Ge, Voss, & Molotch, 2018; Evans, Godsey, Rushlow, & Voss, 2020; Huang et al., 2020; Lamontagne-Hallé et al., 2018), and to a very limited extent presented field applications of these models (e.g., Dagenais et al., 2020; Evans et al., 2020; Kurylyk, Hayashi, Quinton, McKenzie, & Voss, 2016; Langford, Schincariol, Nagare, Quinton, & Mohammed, 2019).

We believe that the use of these new models has been impeded for both applied and theoretical research applications due to the lack of visibility and availability of these codes as well as their apparent complexity. Due to the paucity of cold-regions groundwater data and the emerging scientific and societal questions related to permafrost thaw and hydrologic change, we further believe that there is a need to expand the use of cryohydrogeologic modeling tools to include different scenarios and to assist users in the process of creating and applying their own site-specific models.

The objective of this primer is to provide practical guidelines and suggestions for cryohydrogeologic modeling, with the content targeted at those who have some prior groundwater modeling experience without freeze–thaw processes. Some cryohydrogeologic modeling tools have been further developed to include surface processes adapted to cold regions, but this primer does not address the parameterization of their surface component as we focus on subsurface processes. Figure 2 summarizes the main development steps of each section and provides a framework for this article.

2 | CRYOHYDROGEOLOGIC MODELS

The first mathematical models of water flow in freezing soils were developed in the 1970s, coincident with the economic development of northern regions from the expansion of the oil and gas industry (e.g., Guymon & Luthin, 1974; Harlan, 1973; Kurylyk & Watanabe, 2013; Taylor and Luthin, 1978). In most cases, the partial differential equations for water flow and energy transport for these models were restricted to the vertical dimension due to computational limitations, and as such, these models are not suitable for understanding multi-dimensional groundwater flow systems.

Molson, Frind, and Palmer (1992) accounted for seasonal ground freeze–thaw and advective–conductive heat transfer processes in a 3D model while incorporating temperature-dependent fluid density and fluid viscosity and considering the effects of pore water phase change on the energy balance. McKenzie et al. (2007) enhanced the multidimensional groundwater flow and energy transport simulator SUTRA to include similar dynamics and the effect of pore water phase change on hydraulic conductivity. A series of additional cryohydrogeologic modeling tools with varying physical processes and solution strategies were created shortly afterward (e.g., Bense & Person, 2008; Dall'Amico, Endrizzi, Gruber, & Rigon, 2011; Frampton, Painter, Lyon, & Destouni, 2011; Painter, 2011; Rowland et al., 2011).

Over the last decade, new powerful tools that fully couple surface and subsurface thermal and hydrologic processes have been developed to address the critical importance of cold-regions surface hydrology on hydrogeological systems

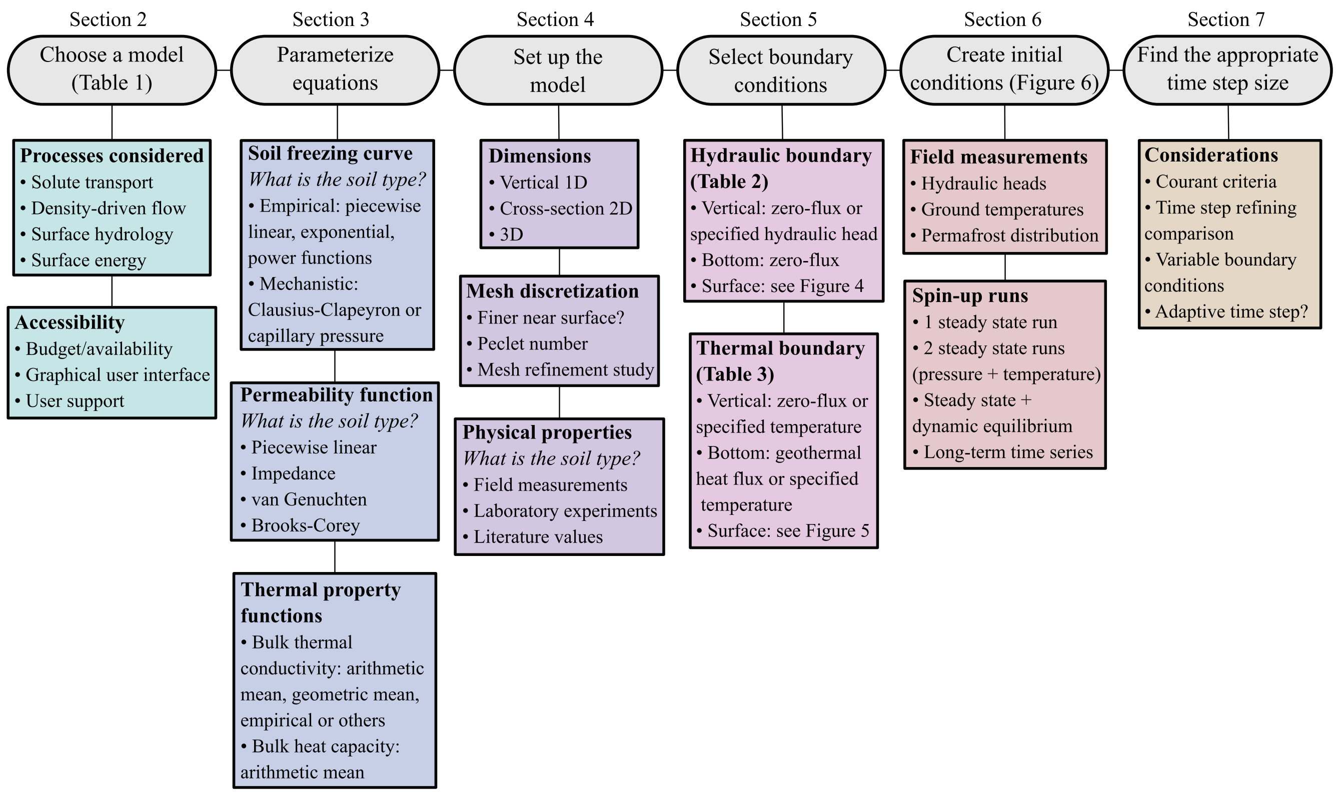


FIGURE 2 Model setup steps for a cryohydrogeologic numerical model

(e.g., Endrizzi et al., 2014; Nitzbon et al., 2019; Painter et al., 2016; Schilling, Park, Therrien, & Nagare, 2019; Zhang, Wen, Xue, Chen, & Li, 2016). These integrated models simulate many surface hydrologic and thermal processes that are specific to cold regions and potentially important to groundwater flow dynamics such as snow accumulation and melt, differential radiation due to slope aspect, overland flow, and surface albedo change; however, this primer primarily focuses on subsurface processes and parameterization.

In an effort to compare and validate the different simulators of groundwater flow and heat transport in cold regions, an international collaborative benchmarking initiative (InterFrost) was launched in 2014 (Grenier et al., 2018). Thirteen codes (Table 1) were tested and compared in multiple benchmarking scenarios (e.g., Kurylyk, McKenzie, MacQuarrie, & Voss, 2014) and it was concluded that only minor discrepancies existed among the different codes (Grenier et al., 2018; Rühaak et al., 2015). While these different models have proven to yield similar results, there is limited knowledge of how representative they would be when applied to natural systems. The characteristics of these different codes are also included in Table 1. The model GeoTop (Endrizzi et al., 2014), which was not part of the InterFrost project, is also included in Table 1. A more complete history of earlier mathematical models is provided by Kurylyk, MacQuarrie, and McKenzie (2014).

A number of cryohydrogeologic models are currently available, and selecting the appropriate code involves many considerations. These models can be divided into three categories (Table 1): Integrated cryohydrologic codes (i.e., models with coupled surface and subsurface processes, Table 1a), cryohydrogeologic codes (i.e., free-standing codes simulating only subsurface processes, Table 1b), and models which implement cryohydrogeologic processes in general-purpose multiphysics modeling environments (Table 1c). When choosing a particular model, it is important to consider the study objectives, including what modeling aspects should be considered as relevant physical processes in the conceptual model (e.g., the number of dimensions, surface water or energy balance routines, and coupled solute transport), as well as the spatial and temporal scale of the study and the desired modeling strategy.

Additionally, one should consider the accessibility of the modeling tools as part of the selection process. While some codes are open-source, others have been commercialized, and others are only available upon request. The user should therefore use the best option according to their budget, their code archiving requirements, and/or capacity to interact with model developers. As others have noted (e.g., Bredehoeft, 2012), the availability of thorough documentation and institutional support for a groundwater modeling platform is critical for the continued application of that code. Thus,

TABLE 1 Comparison of the features included in the different cryohydrogeologic modeling tools, including GeoTop and the 13 codes involved in the InterFrost project

CODE TYPE	MODEL	Variably saturated flow	Density-driven flow	Mass transport	Reactive transport	Surface hydrological model	Surface energy balance	Parallel computing	Availability	Developer	Graphical user interface	Online user support	Reference	Example of application
a) Integrated cryohydrologic models	**ATS**	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Open source	Los Alamos & Oak Ridge National Laboratories (USA)	No	No	Painter et al. (2016)	Schuch et al. (2017)
	GeoTop	Yes	No	No	No	Yes	Yes	Not yet	Open source	University of Zurich (Switzerland) & Eurac Research (Italy)	No	Yes	Endrizzi et al. (2014)	Fullhart et al. (2018)
b) Free-standing cryohydrogeologic models	**DarcyTools**	Yes	Yes	Yes	No	No	No	Yes	Upon request	Swedish Nuclear Fuel and Waste Management Co (Sweden)	No	No	Svensson et al. (2010)	Svensson and Ferry (2014)
	FEFLOW	Yes	Yes	Yes	Yes	With Mike11	No	Yes	Commercial license only	DHI Group	Yes	Yes	DHI (2016)	Langford et al. (2019)
	GEOAN	Yes	Yes	Yes	No	Yes	No	Yes	Unknown	Golder Associates	No	No	Holmén et al. (2019)	Holmén et al. (2011)
	Ginette	No	No	No	No	Yes	No	No	Unknown	MINES ParisTech (France)	No	No	Rivière et al. (2019)	Rivière et al. (2019)
	MELT	No	Yes	Yes	No	No	No	No	Unknown	Desert Research Institute (USA)	No	No	Frederick and Buffet (2014)	Frederick and Buffet (2016)
	PFLOTRAN	Yes	Yes	Yes	Yes	Not yet	No	Yes	Open source	Los Alamos & Sandia National Laboratories (USA)	No	Yes	Karra et al. (2014)	Kumar et al. (2016)
	SMOKER	No	Yes	Yes	With CHEAT	No	Boundary layer	No	Open source	Université Laval & University of Waterloo (Canada)	No	No	Molson and Frind (2019)	Dagenais et al. (2020)
	SUTRA	Yes	Yes	No	No	Surface water mass balance	Not yet	No	Upon request (soon online)	United States Geological Survey (USA)	ArgusOne (license needed)	No	McKenzie et al. (2007)	Lamontagne-Hallé et al. (2018)
c) General multiphysics modelling environments	Implementation in **Cast3M**	Yes	No	Yes	No	Yes	No	No	<u>Imp.</u> Unknown <u>Platform</u> Free for research	<u>Imp.</u> LSCE (France) <u>Platform</u> CEA (France)	No	Yes	Roux et al. (2017)	Grenier et al. (2013)
	COMSOL	Yes	Yes	Yes	Yes	Yes (no snow)	Yes (no snow)	Yes	Commercial license only	COMSOL Group	Yes	Yes	Scheidegger et al. (2017)	Scheidegger et al. (2019)
	Implementation in **FlexPDE**	No	No	No	No	No	No	Yes	<u>Imp.</u> Unknown <u>Platform</u> Commercial license	<u>Imp.</u> University of East Anglia (UK) <u>Platform</u> PDE Solutions	Yes	Yes	Bense et al. (2009)	Bense et al. (2012)
	PermaFoam (Implemented in OpenFOAM)	Yes	No	No	No	Evapo-transpiration	No	Yes	<u>Imp.</u> Open source <u>Platform</u> Open source	<u>Imp.</u> Université Paul Sabatier (France) <u>Platform</u> OpenCFD Ltd.	No	No	Orgogozo et al. (2019)	Orgogozo et al. (2019)

new cold-regions groundwater modelers should invest their time in a code with support. One should also consider the usability, flexibility, and ease of modifiability of the code as well as the availability of a graphical user interface for preprocessing and postprocessing. A list of information about some of the modeling options is presented in Table 1 to aid in the decision-making process. It should be noted that the numerical approach used to solve the governing equations can be unique for every code and may be of critical importance to produce reliable results (see Grenier et al., 2018).

3 | GOVERNING EQUATIONS AND CHARACTERISTIC FUNCTIONS

Cryohydrogeologic models solve at least two coupled governing equations: a groundwater flow equation and an energy transport equation. A select few also consider coupled solute transport (e.g., Frederick & Buffett, 2016; Molson & Frind, 2019). Other codes (e.g., Nishimura, Gens, Olivella, & Jardine, 2009) also include geomechanical processes, but these are more commonly developed and applied for cold-regions geotechnical engineering and are outside the scope of this primer. The applied groundwater flow equation is usually a multi-dimensional form of Darcy's equation that may include unsaturated flow or density-dependent flow. The energy transport equation describes heat transfer through conduction and advection (heat transfer induced by the movement of a fluid) in a porous medium as well as the latent heat released or absorbed during soil freeze–thaw. These two coupled equations are predicated on the conservation principles of fluid mass and energy. Based on these coupled equations, the model calculates the pressure (or hydraulic head) and temperature distributions throughout the discretized model domain (Figure 3). While the governing equations themselves are similar for most models, they vary greatly in their coupling approach (referred to as the thermo-hydrologic coupling), or, in other words, how the pressure solution influences the temperature solution and vice versa.

The unique feature of cryohydrogeologic models is their ability to represent, within both of the governing equations, dynamic freezing, and thawing processes due to pore water phase change. This creates important feedback between the energy transport equation and the groundwater flow equation (Figure 3). Once the temperature drops below a certain reference temperature, usually close to 0°C, pore water may begin to freeze. During cooling, the temperature at which freezing is initiated depends on the type of soil, its water saturation, pressure, and the water solute concentration (Kurylyk & Watanabe, 2013). Some modeling tools use modified versions of the Clausius–Clapeyron equation to find the freezing point of water depending on the pressure conditions (e.g., Dall'Amico et al., 2011; Painter & Karra, 2014), while others require the freezing point to be defined by the user by varying a parameter of the soil freezing curve described below. Below the freezing point temperature, the surface energy of the soil particles maintains a certain quantity of liquid water, which will continue to decrease with temperature (Wang, Lai, & Zhang, 2017). Transitioning from a porous medium composed of soil particles, liquid water, and air, to one that also includes ice, strongly impacts the hydrogeological and thermal properties. First, the formation of pore ice will drastically decrease a porous medium's permeability or hydraulic conductivity (Watanabe & Osada, 2016). Second, due to the difference in the thermal properties

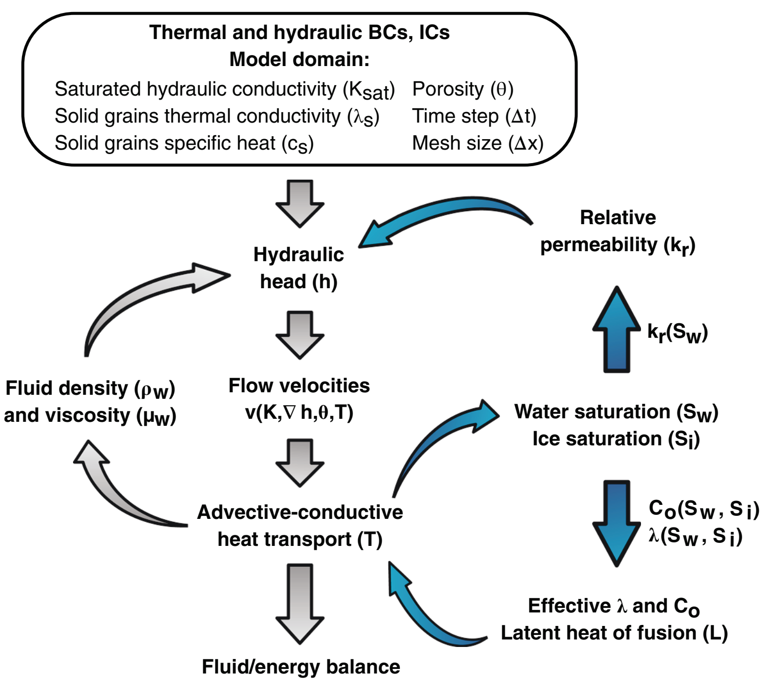


FIGURE 3 Basic structure of a cryohydrogeologic model, showing primary links between flow and heat transport modules solving for heads (h) and temperature (T), respectively, with freeze–thaw processes represented by blue arrows. BCs and ICs stand for boundary conditions and initial conditions, respectively, and C_o and λ stand for the bulk heat capacity and bulk thermal conductivity of the porous medium, respectively

of ice and water, pore water phase change will increase the bulk thermal conductivity and decrease the heat capacity of the soil. Finally, the freezing or melting of pore water will respectively release or absorb energy through latent heat.

Functions must be defined which describe the interplay between ground temperatures, freezing processes, and hydrogeologic parameters. This is typically accomplished by adding additional terms and associated parameters to the governing energy and mass (water) balance equations. There are three common relationships, specific to cryohydrogeologic models, that must be defined:

1 *The Soil Freezing Curve* calculates liquid water saturation from computed subfreezing temperature. A soil does not fully freeze at 0°C, but rather freezing and thawing occurs over a temperature range. Generally, this range is larger for fine-grained soils, and smaller for coarse-grained soils (Watanabe, Kito, Wake, & Sakai, 2011), and is analogous to the unfrozen soil moisture curve that describes soil drying over a range of negative pore-water pressures. Cryohydrogeologic models have employed many different soil-freezing functions which can be separated into two categories: Empirical and mechanistic approaches. The empirical approach relies on a predefined function for which the parameters are estimated from laboratory measurements. The chosen functions are usually a piecewise linear function (McKenzie et al., 2007), a power function (Kurylyk et al., 2016), or an exponential function (Evans et al., 2018; Mottaghy & Rath, 2006; Shojae Ghias et al., 2018). These empirical approaches usually require one or two empirical fitting parameters, such as a slope or an exponent, to describe the decrease in liquid water content as temperatures are lowered.

   The mechanistic approach consists of establishing the soil freezing curve from the unfrozen soil moisture curve calculated from the van Genuchten analytical model (van Genuchten, 1980) or a related expression, and by replacing the matrix suction term by a form of the Clausius–Clapeyron equation (Dall'Amico et al., 2011; Hansson, Šimůnek, Mizoguchi, Lundin, & van Genuchten, 2004; Sheshukov & Nieber, 2011). This equation defines the pressure and temperature conditions at which two phases may coexist. This method allows for a freezing point temperature dependent on pressure conditions (i.e., freezing point depression), but usually assumes that surface tensions at the ice–liquid and air–liquid interface are the same. Using a similar approach but without the aforementioned assumption, Painter and Karra (2014) developed a complex set of equations for unsaturated soils that integrates the effect of capillary pressure and a flexible dependence on the total water content. When parameterizing the soil freezing function, often a residual or minimum water content limit is set (McKenzie et al., 2007; Shojae Ghias et al., 2018) that prevents the soil from freezing completely. Readers are directed to Watanabe and Osada (2016), Watanabe and Osada (2017), and Teng, Kou, Yan, Zhang, and Sheng (2020) for examples of laboratory measurements of different soils as well as Kurylyk and Watanabe (2013) and Amiri, Craig, and Kurylyk (2018) for a more detailed description of soil freezing curves.

2 *The Permeability Function* determines the permeability based on the liquid water saturation. As the ice saturation increases (i.e., during freezing) and/or when the water saturation decreases due to draining, the permeability will decrease by up to several orders of magnitude. There are many possible permeability functions, and the choice of function and parameterization should be in accordance with prior lab or field studies conducted for specific soil types (Burt & Williams, 1976). Some past studies have used empirical functions such as a linear decrease in permeability with liquid saturation (Grenier et al., 2013; Kurylyk et al., 2016) or the use of an impedance factor (Evans & Ge, 2017; Hansson et al., 2004; Lundin, 1990) which exponentially decreases the permeability with decreasing temperature (or increasing pore ice saturation) until a certain minimum permeability has been reached.

   Other cryohydrogeologic modeling studies have integrated the van Genuchten (1980) equation representing the soil freezing curve into the Mualem (1976) model (Karra et al., 2014; Schuh et al., 2017). While not required, the van Genuchten equation is usually preferred to calculate permeability if it is also used for the soil freezing curve. Like the popular Brooks–Corey equation (Brooks & Corey, 1966; Sheshukov & Nieber, 2011), the van Genuchten equation requires two fitting parameters which can be calibrated from experimental data or estimated from existing models (e.g., Ghanbarian-Alavijeh, Liaghat, Huang, & van Genuchten, 2010; Schaap, Leij, & van Genuchten, 2001) or databases (e.g., Montzka, Herbst, Weihermüller, Verhoef, & Vereecken, 2017; Schaap & Leij, 1998). A calibrated impedance factor may be added to account for flow restrictions caused by the ice blockage of pores (Dall'Amico et al., 2011; Sheshukov & Nieber, 2011), although Painter (2011) demonstrated that it was not necessary. In most cases, these equations determine the medium's "relative permeability", which is the ratio of the actual permeability of a frozen, and potentially partly unsaturated, medium, to the unfrozen, saturated permeability. Examples of laboratory measurements are given by McCauley, White, Lilly, and Nyman (2002), Watanabe and Osada (2016), and Watanabe and Osada (2017). Kurylyk and Watanabe (2013) provide a detailed analysis of the different permeability functions.

3 *The Thermal Property Functions* describe the change in bulk thermal conductivity and bulk heat capacity as a function of ice saturation. Generally, it is assumed that ice has a thermal conductivity between 2.1 and 2.4 J m^{-1} $s^{-1\circ}C^{-1}$ and a specific heat capacity between 1,800 and 2,100 J $kg^{-1\circ}C^{-1}$, while liquid water has a thermal conductivity of between 0.54 and 0.60 J m^{-1} $s^{-1\circ}C^{-1}$ and a specific heat capacity between 4,180 and 4,190 J $kg^{-1\circ}C^{-1}$ (e.g., Bense et al., 2012; Grenier et al., 2018; McKenzie et al., 2007; Williams & Smith, 1989). Therefore, with freezing, the ratio of the volumetric contributions of ice and water changes, requiring a recalculation of the bulk thermal conductivity and heat capacity. Heat capacity is not directional, and thus the bulk heat capacity is often calculated as the arithmetic mean of the individual constituents (air, ice, water, and soil particles) weighted by their individual volumes (e.g., Bense et al., 2009; McKenzie et al., 2007). In contrast, thermal conductivity is a directional tensor, and thus different averaging methods have been employed, with two common approaches being the arithmetic (e.g., McKenzie et al., 2007; Shojae Ghias, Therrien, Molson, & Lemieux, 2017) and geometric means (e.g., Scheidegger et al., 2017) weighted by the respective constituent volumes. While not always accurate (Buntebarth & Schopper, 1998), the weighted geometric mean is generally more accurate than the arithmetic mean (Fuchs, Schütz, Förster, & Förster, 2013; Zhang, Lu, Lai, & Zhang, 2018) and can provide reasonable estimates of bulk thermal conductivities if the thermal conductivities of each individual constituent are within the same order of magnitude (Ghanbarian & Daigle, 2016; Jorand, Fehr, Koch, & Clauser, 2011; Nield & Bejan, 1999).

Some codes use a semi-empirical method from Johansen (1975) that requires either the thermal properties of the dry, saturated unfrozen, and saturated frozen soils (Karra et al., 2014) or those of each individual soil component (Painter, 2011). The Johansen method calculates the bulk thermal conductivity from the thermal conductivities of the dry, saturated unfrozen and saturated frozen soil weighted by two normalized thermal conductivities, known as the Kersten numbers for frozen and unfrozen conditions. A Kersten number (Kersten, 1949) represents the ratio of partially saturated thermal conductivity to fully saturated thermal conductivity and is calculated as the ice or liquid water saturation raised to an empirical exponent. Johansen (1975) further developed empirical functions to estimate dry and saturated unfrozen thermal conductivities from soil properties. This method has shown to provide very good estimates of bulk thermal conductivities for natural soils with a saturation of 20% or higher (Farouki, 1982; Peters-Lidard, Blackburn, Liang, & Wood, 1998), but is not as accurate for dry soils (Fricke, Misra, Becker, & Stewart, 1992).

4 | MODEL SETUP

In general, the computational demand associated with cold-regions groundwater modeling can be prohibitive as the codes typically require (a) smaller time steps and a fine mesh due to the nonlinear nature of the groundwater flow equation with hydraulic conductivities that vary by several orders of magnitude and (b) longer simulation times to understand the hydrogeological impacts of future climate warming and permafrost thaw. Due to these computational requirements, one and two-dimensional models have to date been far more commonly employed for cold-regions groundwater systems than three-dimensional models. Jan, Coon, Painter, Garimella, and Moulton (2018) demonstrated that, with the appropriate approach, one- and two-dimensional cold-regions subsurface models may be as representative of some cold-regions settings as three-dimensional models. Two-dimensional models of cold-regions groundwater systems should always be developed in a vertical cross-section as aerial models do not have the depth-dependent information that is critical in permafrost settings to represent the vertical movement of groundwater flow and the freeze–thaw front.

Most cryohydrogeologic codes cited in Table 1 offer the option of creating three-dimensional models, which may be required to understand the potential effect of heterogeneity (Painter et al., 2016). Three-dimensional models have been applied before (e.g., Evans et al., 2020; Jan, Coon, & Painter, 2019; Karra et al., 2014; Langford et al., 2019) and the theory behind them does not differ from two-dimensional models. However, due to the lack of developed graphical user interfaces for most cryohydrogeologic modeling tools, three-dimensional models can be challenging to create and parameterize. More importantly, three-dimensional models require more computational resources due to the large number of nodes.

The model domain size and mesh discretization should be carefully chosen to best represent the system scale and to allow accurate reproduction of heterogeneities and hydraulic and thermal gradients while keeping in mind the study's objectives. For example, recent publications have shown the importance of shallow supra-permafrost groundwater on cold-regions hydrology (Lamontagne-Hallé et al., 2018; O'Connor, Cardenas, Neilson, Nicholaides, & Kling, 2019; Rey, Walvoord, Minsley, Rover, & Singha, 2019; Toohey, Herman-Mercer, Schuster, Mutter, & Koch, 2016). To simulate these local processes included in a larger groundwater system, while limiting computational time, a finer mesh size near the surface and a coarser mesh size at greater depths can be used (e.g., McKenzie & Voss, 2013). In general, the shallow subsurface (active layer) experiences seasonal freeze–thaw and normally includes an unsaturated zone which should be discretized more finely to accommodate these dynamic changes. Some modeling tools use an adaptive refinement method which will refine or coarsen the mesh automatically based on the desired precision throughout the simulation (e.g., Diersch, 2014; Orgogozo et al., 2019).

To avoid numerical dispersion, the Peclet criterion (P, dimensionless), the ratio of heat advection to heat conduction, should be respected (Daus, Frind, & Sudicky, 1985). For thermal transport, the Peclet criterion of a one-dimensional system can be calculated as:

$$P = \frac{v\,\Delta x}{\frac{\lambda}{\theta S_w c_w \rho_w} + D} \leq 2 \tag{1}$$

where v is the magnitude of the computed groundwater velocity (m s^{-1}), Δx is the element size (m), λ is the bulk thermal conductivity of the porous medium (J m^{-1} s$^{-1\circ}$C^{-1}), θ is the porosity (–), S_w is the water saturation (–), and ρ_w and c_w are the liquid water density (kg m^{-3}) and specific heat capacity (J kg$^{-1\circ}$C^{-1}), respectively. The hydrodynamic dispersion term D (m^2 s^{-1}) is added for completeness; it is often neglected in thermal transport since it is usually much less than the thermal diffusivity (Bear, 1972). Dispersivities for the dispersion coefficient can be estimated from the system scale (e.g., Schulze-Makuch, 2005; Xu & Eckstein, 1995). To minimize errors, a "mesh refinement study" should be performed by increasing the mesh or grid density until no significant difference in the model outcomes exists (e.g., Lamontagne-Hallé et al., 2018; McKenzie et al., 2007; Orgogozo et al., 2019).

Once the domain is established and discretized, model parameters are assigned, including any spatial variability in parameter values. In addition to the properties of typical groundwater models, such as the saturated hydraulic conductivity (or permeability) and porosity, the user must assign parameters for the relative permeability function, soil freezing curve, specific heat (heat capacity/density), thermal conductivity, and density of every phase (i.e., solid particles, liquid water, ice, and air). These can be estimated from field measurements, laboratory experiments, or literature values (e.g., O'Connor et al. (2020), Williams and Smith (1989) or any online data portal, such as the NGEE-Arctic website, http://ngee-arctic.ornl.gov for soil properties values). Albers, Molson, and Bense (2020), Ebel, Koch, and Walvoord (2019), Harp et al. (2015), Zipper, Lamontagne-Hallé, McKenzie, and Rocha (2018) and others provide more information on the importance of these parameters in cryohydrogeologic models. Other parameters such as the latent heat of fusion (334,000 J kg^{-1}), compressibility, and dispersivity may also need to be set. When conducting unsaturated zone simulations, one should also carefully consider the parameterization of the model's soil-water characteristic curve and unsaturated permeability function and how these relate to the soil freezing curve and relative permeability function for pore water phase change.

5 | BOUNDARY CONDITIONS

While the governing equations effectively define the processes occurring within the model domain, the boundary conditions (BCs) define the system conditions and fluxes into and out of the model domain. For cryohydrogeologic models, every part of each model boundary must include boundary conditions for both groundwater flow and thermal transport.

5.1 | Hydraulic boundary conditions

A hydraulic BC controls the hydraulic conditions (e.g., pressure or water fluxes) at a boundary and can be seen as a gate for water to enter and/or exit the model, or as an impermeable barrier to prevent water flow across a boundary.

Different hydraulic BCs are available depending on the model employed (Table 2). In most models, the user can specify a constant or time-varying pressure or hydraulic head at hydraulic boundary nodes (Dirichlet type), the water flux that crosses this boundary (Neumann type), or a relationship in which a water flux is calculated from the pressure or head value at the boundary (Cauchy-type). Often cold-regions groundwater models are intended to represent the groundwater system underlying a surface watershed; therefore, a common assumption is to set the vertical hydraulic BCs as no-flow conditions along the watershed boundaries. A similar no-flow assumption is often invoked at the base of the model, which is often placed deep enough to reach unfractured bedrock or any layer in which the permeability is too low to produce any significant groundwater flow compared to the shallower layers. A lower no-flow BC may be placed at shallower depths in permafrost settings, provided that the lower boundary remains frozen and effectively impermeable throughout the simulation (e.g., McKenzie et al., 2007). A common rule-of-thumb is that a no-flow boundary is justified at a hydrostratigraphic interface if the hydraulic conductivity contrast across the interface is at least two orders of magnitude (Anderson, Woessner, & Hunt, 2015).

Assigning an appropriate BC at the surface can be more challenging for groundwater modeling in cold regions. The main difference in choosing a surface BC for a typical groundwater model versus a cryohydrogeologic model resides in the complex surface processes occurring in cold regions and in the changing ground properties due to freeze–thaw. A common approach in groundwater modeling is to assign the surface boundary conditions according to its context as either representing a recharge zone or a discharge zone (usually where a water body is observed at the surface; Anderson et al., 2015). A Neumann-type BC in the recharge zones (water input) and a Dirichlet-type in the discharge zones could be set, with the assigned pressure or hydraulic head corresponding to the water level in the surface water body. However, due to the pronounced changes in hydraulic conductivity induced by the freezing or thawing of the active layer and the lowering of the permafrost table, these delimited recharge and discharge zones likely change seasonally and at longer time scales in response to climate warming (Cooley, Smith, Ryan, Pitcher, & Pavelsky, 2019; Walvoord, Voss, & Wellman, 2012; Yoshikawa & Hinzman, 2003), making this approach potentially overly constrained for modeling cold regions.

The simplest model setup is to assume full saturation in the model and specify the water table at the model domain surface with a Dirichlet-type BC based on the topography (Figure 4a). This approach was implemented in many studies (e.g., Bense et al., 2012; Ge, McKenzie, Voss, & Wu, 2011; McKenzie & Voss, 2013). When field data are available, one could use a hydraulic Dirichlet BC corresponding to the measured hydraulic head in both fully and partially saturated conditions (Figure 4b; Shojae Ghias et al., 2017; Zipper et al., 2018). This approach has the advantage of self-regulating the water flux at the boundary based on the ground conditions, meaning that the flux will decrease as the ground freezes since its hydraulic conductivity decreases as well. However, as acknowledged by Ge et al. (2011) and McKenzie and Voss (2013), using a Dirichlet BC assumes that an unlimited quantity of water can enter or exit the model through this boundary. This approach may thus potentially greatly overestimate groundwater recharge, flow, and groundwater discharge, and can overestimate permafrost thawing rates through heat advection. With a fixed hydraulic head, one should always verify that the model-computed fluxes are reasonable, especially those across the top model surface. Fixing the hydraulic head is not useful if the purpose of the model is to simulate the potential shifts in the water table caused by climate-driven changing precipitation regimes or the vertical movement of the freezing front and the permafrost table. To avoid the negative feedback of using a land-surface specified pressure BC, Evans et al. (2018) and Lamontagne-Hallé et al. (2018) coupled a time-dependent Neumann type BC that specifies the groundwater recharge from precipitation and snowmelt (Figure 4d) with a drain BC (Cauchy type, Figure 4c). The drain boundary condition removes water when pressures at a given model location exceed a given value—at the land surface, this is assumed to be 0 Pa. This approach allows discharge from the model at any over-pressurized surface nodes without drawing any water into the domain like a specified pressure BC would (Figure 4c). In addition to preventing unreasonable water input at the surface, this combination of BCs used with variable saturation conditions can simulate water table variations as permafrost thaws and can also represent dynamic seasonal or long-term changes to groundwater recharge. The drain BC can also be modified to represent a lake or a river that could receive or release water depending on the pressure conditions at the water body bed (Figure 4d).

For a more detailed consideration of surface processes, the user could link a groundwater model with an external surface water model to fully consider evapotranspiration, groundwater-surface water exchanges, snowmelt, and canopy layers (Figure 4e; e.g., Langford et al., 2019). Typically, a "one-way coupling" approach is used in which the surface model is first run independently of the groundwater model, and the surface model output (e.g., infiltration or groundwater recharge) is then used to drive the groundwater model at the land surface. This approach does not allow the groundwater model to exert control on the surface water model. Any limitations of "one-way coupling" can be avoided

TABLE 2 Typical hydraulic boundary conditions used in cryohydrogeologic modeling studies

Boundary	Description	Type	Time dependency	Water in or out	Used to represent	Considerations	Assumptions	Used in
Vertical (sides)	Zero water exchange (Figure 4a,4c,4d,4e)	Neumann	Constant	None	Watershed limits	• Watershed limits	• Vertical boundaries are at the limits of a watershed • The groundwater watershed limits are static and fit with the surface watershed limits	Bense et al. (2012)
	Fixed hydraulic heads (Figure 4b)	Dirichlet	Constant or variable	Both	Non-watershed limits Seepage face	• Water exchange with the surroundings	• Future pressure conditions at all points of the boundary are known • Changes of pressure in depth are known at all points of the boundary	Shojae Ghias et al. (2017)
Base	Zero water exchange	Neumann	Constant	None	Deep impermeable bedrock or permafrost	• Deep impermeable layer	• Base of the model is impermeable to groundwater flow • If used to represent permafrost, the model base will stay frozen and impermeable for the duration of the simulation • Regional groundwater flow contribution is not significant	McKenzie et al. (2007)
Surface (top)	Zero specified pressure at the surface (Figure 4a)	Dirichlet	Constant	Both	Land surface Water bodies	• Fully saturated flow	• Model always stay fully saturated • An unlimited amount of water is available to keep the model saturated • No signifant water ponding occurs at the surface	McKenzie and Voss (2013)
	Surface specified hydraulic head (Figure 4b)	Dirichlet	Constant or variable	Both	Land surface Water bodies	• All surface processes	• Hydraulic head field measurements are available and are representative of the model domain surface • Future trends of water table variations are known	Shojae Ghias et al. (2017)
	Constant specified recharge (Figure 4c)	Neumann	Constant	Water input only	Land surface	• Unsaturated and saturated flow • Limited amount of water available	• Groundwater recharge is known and constant over time • Water infiltation occurs even if the ground is frozen	Evans and Ge (2018)
	Seasonally variable specified recharge (Figure 4d)	Neumann	Variable	Water input only	Land surface	• Unsaturated and saturated flow • Snowmelt recharge • Recharge variations • Limited amount of water available	• Water input during the snow-free season is known • Water input due to snowmelt during freshet is known • Recharge during the freezing season is null • Evapotranspiration and vegetation are negligible	Lamontagne-Hallé et al. (2018)
	Drain (Figure 4c) (Qout α Pressure)	Cauchy	Constant or variable	Water output only	Land surface	• Overland flow if saturated	• Relationship between water output and pressure is known • No significant water ponding occurs at the surface	Evans and Ge (2018)
	One-way coupling with external surface model (Figure 4e)	Neumann or Dirichlet	Variable	Both	Land surface Water bodies	• All the surface processes included in the surface model	• Atmospheric, land surface and canopy layer conditions are known including future trends • Subsurface conditions do not have any effect on the surface conditions	Langford et al. (2019)
	Two-way coupling with internal equations (Figure 4e)	Built-in function	Variable	Both	Land surface Water bodies	• All the surface processes included in the surface model • Effects of subsurface conditions on surface conditions	• Atmospheric, land surface and canopy layer conditions are known, including their future trends	Jafarov et al. (2018)

Note: The "Used in" column provides one study example for each boundary condition.

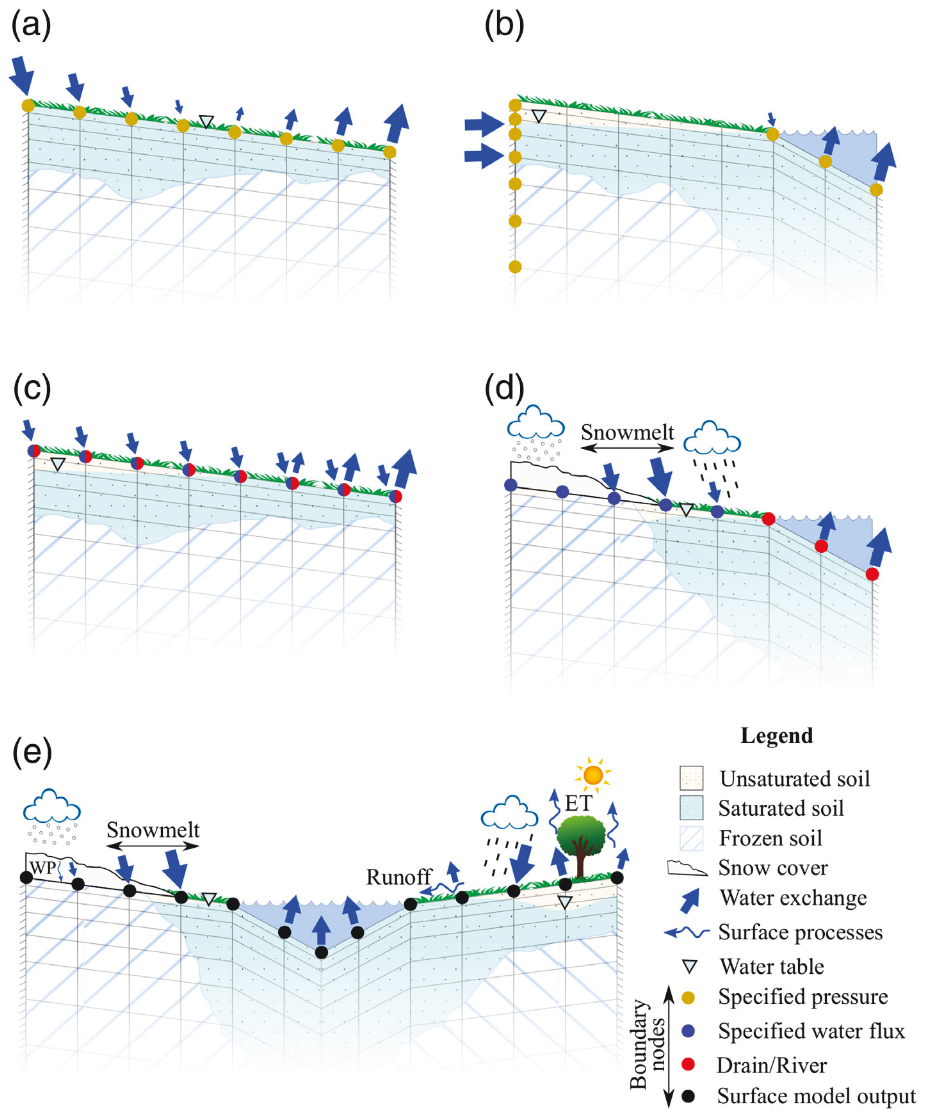


FIGURE 4 Conceptual model of typical surface hydraulic boundary condition configurations for cryohydrogeologic numerical models: (a) surface-specified hydraulic head; (b) specified hydraulic head on the left boundary and under the water body; (c) constant specified recharge coupled with a drain; (d) seasonally variable specified recharge with drain nodes under the water body; (e) specified water inflow/outflow or head/pressure from a linked surface hydrological model. ET is evapotranspiration and WP is water percolation through the snow cover

by using a built-in surface water model, such as the surface routines incorporated in the integrated cryohydrologic models such as ATS and GeoTop (Table 1a, Endrizzi et al., 2014; Painter et al., 2016), or in the HydroGeoSphere model (e.g., Schilling et al., 2019). These may also include a snow model to simulate snow-related processes potentially impacting the hydrogeological system such as water percolation in a snow layer and infiltration in frozen soils (Ireson, van der Kamp, Ferguson, Nachshon, & Wheater, 2013; Iwata, Hayashi, Suzuki, Hirota, & Hasegawa, 2010; Maurer & Bowling, 2014).

In any case, the user should carefully consider the realism of the BC combinations before running a model. The choice of surface BCs should partly depend on the side and base BCs, and vice versa. For example, if no-flow boundaries are used for the sides and the base of the model, the surface cannot be exclusively a Neumann-type BC. Otherwise, the simulation will likely produce unrealistic pressure conditions. In this case, a few Dirichlet-type or drain BC (Cauchy-type) nodes, for which the water flux crossing the boundary is dependent on the modeled head or pressure conditions, are necessary.

5.2 | Thermal boundary conditions

Most modeling studies of heat transport in groundwater systems use two types of thermal BCs (Table 3): A specified temperature BC (Dirichlet type), which allows a model-derived heat flux into or out of the model, and a specified heat flux (Neumann-type), which defines the exact heat flux entering or leaving the domain. Cryohydrogeologic models often include a geothermal heat flux assigned at the base of the model domain (for example, usually between 30 and 100 mW m^{-2}, see Majorowicz and Grasby (2010) and Batir, Blackwell, and Richards (2016) for geothermal heat flow maps of Canada and Alaska, respectively). The geothermal heat flux is very site specific, and the temperature gradient of permafrost systems can be distorted due to their memory of past climates (Isaksen, Mühll, Gubler, Kohl, & Sollid, 2000). Its value should be chosen considering the geographical location of the modeled site rather than using a regional average. If a geothermal flux condition is applied over long time scales, the lower boundary should extend to many hundreds of meters to avoid the effect of past climates. If borehole temperature measurements are available, one could alternatively use a specified constant temperature BC at the domain base, as long as it is reasonable to assume that land surface warming signals will not penetrate to the domain base (e.g., Atchley et al., 2015; Rushlow, Sawyer, Voss, & Godsey, 2020; Zipper et al., 2018). Similar to the hydraulic BCs, the vertical domain boundaries are often considered to have no heat exchange since they usually correspond to the limits of a watershed, resulting in no lateral water flow (thus no heat advection) and horizontal isotherms (thus no lateral thermal conduction). The Global Terrestrial Network for Permafrost database (http://gtnpdatabase.org/) provides some information on cold-regions subsurface temperature measurements that could aid in boundary condition parameterization.

Different options have been proposed in the literature to represent the surface thermal boundary condition (Table 3). This domain boundary represents the location of the primary thermal forcing in response to climate change. Many cold-region surface processes, such as snow cover insulation, snow redistribution, shifts in vegetation, differential radiation due to slope aspect, turbulent fluxes, and seasonally variable albedo, significantly impact the ground thermal and hydrologic conditions (Jorgenson et al., 2010; Shur & Jorgenson, 2007; Young, Lemieux, Delottier, Fortier, & Fortier, 2020). Depending on the setting, some of these processes strongly influence land surface temperatures (Goodrich, 1982; Zhang, 2005), which in turn will impact the distribution of frozen ground and groundwater flow patterns (Connon, Devoie, Hayashi, Veness, & Quinton, 2018; Huang et al., 2020; Kurylyk, MacQuarrie, & McKenzie, 2014; Qi et al., 2019). For example, O'Neill and Burn (2017) found that a talik had formed underneath a snow fence in continuous permafrost, which led to half a meter of land subsidence. Jan and Painter (2020) used ATS to simulate the effects of snow accumulation timing on permafrost thermal conditions and found that even a small shift can affect the active layer thickness. Integrated cryohydrologic codes (e.g., ATS and GeoTop, Table 1a) consider some of these processes with a surface energy balance and a snow distribution model fully coupled to their subsurface components. CryoGrid 3 xIce (Nitzbon et al., 2019) also simulates these surface processes, but is not considered here as a cryohydrogeologic model because processes such as vertical groundwater flow, permeability dependence on liquid saturation and heat advection are neglected. For a full consideration of surface thermal processes and their interactions with the subsurface, one may use the built-in options offered in these tools.

However, a surface energy balance module requires extensive parameterization data, and such modules are often not available in cryohydrogeologic models. The user may instead need to choose a surface thermal BC. The decision should be made by first considering the studied environment and its driving factors, the study objectives, and the availability of field data (Table 3). If surface temperature data are available, an ideal solution that considers all the processes listed above is to assign the measured surface temperatures as a specified temperature BC (Dirichlet type; Figure 5a). On the other hand, this approach, which has been used in many studies (e.g., Bense et al., 2009; Ge et al., 2011; Sjöberg et al., 2016), may be problematic once applied to long-term climate warming scenarios. Ground surface temperature projections are often unknown or uncertain and highly dependent on the ground conditions (Mann & Schmidt, 2003). In particular, snowpack evolution may decouple long-term trends in air and surface temperatures (Kurylyk, Bourque, & MacQuarrie, 2013; Mellander, Löfvenius, & Laudon, 2007). If ground surface temperatures are unknown, one can use "n-factors" as an estimation (Lunardini, 1978). The n-factor approach, as used in Fortier, LeBlanc, and Yu (2011) and Walvoord, Voss, Ebel, and Minsley (2019), is the ratio of cumulative ground surface temperature to air temperature degree-days. However, n-factors are site-specific and depend on surface conditions, for example, if snow cover is present. Additional physical equations may also be used, such as those proposed by Williams et al. (2015) which consider radiative, conductive, sensible, and latent heat to estimate ground surface temperatures in snow-free conditions.

Since air temperature projections are easily accessible from climate models, McKenzie et al. (2007) assigned air temperatures as a specified temperature BC on top of a 1 m thick "thermal boundary layer" with a calibrated thermal

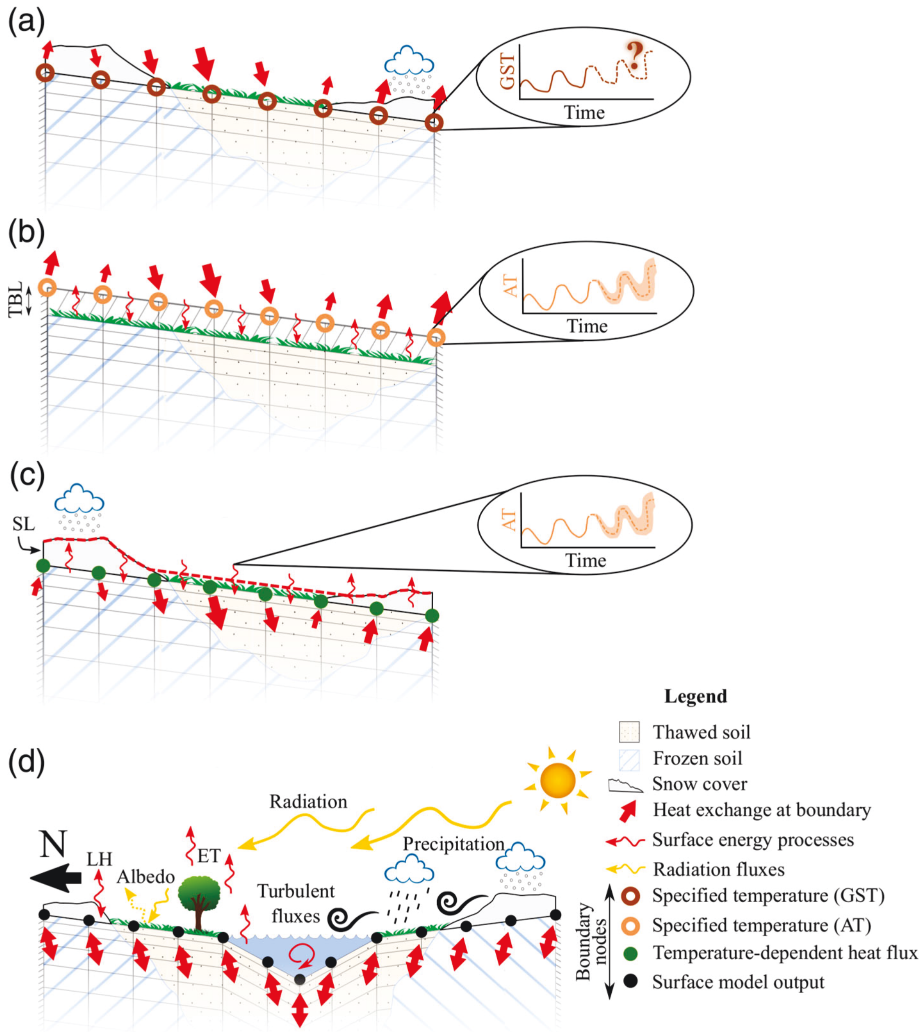
TABLE 3 Typical thermal boundary conditions used in cryohydrogeologic modeling studies

Boundary	Description	Type	Time dependency	Heat in or out	Used to represent	Considerations	Assumptions	Used in
Vertical (sides)	Zero heat exchange	Neumann	Constant	None	Watershed limits	• Watershed limits	•Vertical boundaries correspond to watershed boundaries thus no heat advection from lateral flow • Horizontal isotherms (no conductive heat transfer with the neighbouring watershed)	McKenzie et al. (2007)
	Specified temperature	Dirichlet	Variable	Both	Profile with temperature data	• Heat exchange with the surroundings	• Future and current temperature conditions at all points of the boundary are known • Changes of temperature in depth are known at all points of the boundary	Sjöberg et al. (2016)
Base	Specified heat exchange	Neumann	Constant	Heat input only	Source of geothermal heat	• Constant geothermal heat	• Local geothermal heat flux or gradient is known and constant over time and space • No other source of heat under model base • No heat advection through vertical flow	Bense et al. (2009)
	Specified temperature	Dirichlet	Constant	Both	Layer unaffected by surface thermal variations	• Exact thermal state of the model base	• Temperature at the boundary is not affected by seasonal and yearly changes in LS temperatures • Temperature condition at the model base is known at all points	McKenzie et al. (2007)
Surface (top)	Constant specified temperature	Dirichlet	Constant	Both	Deep water bodies	• Differential temperature at the bed of surface water bodies	• Temperature at the water body bed is constant and known • Air temperature variations do not affect the thermal condition of the water body bed • In a river, no heat advection at the riverbed	McKenzie et al. (2007)
	Water body bed specified temperature	Dirichlet	Variable	Both	Water bodies	• Temperature variations with time and water depth at the water bodies bed	• Temperature at the water body bed follows a defined function with time and water depth • Air temperature variations do not affect the thermal condition of the water body bed • In a river, no heat advection at the riverbed	Wellman et al. (2013)
	LS specified temperature (Figure 5a)	Dirichlet	Variable	Both	LS	• All surface processes affecting the LS	• LS temperatures and their projections are known at all points of the boundary • Future ground thermal condition does not have any effect on the LS temperatures	Bense et al. (2009)
	Specified air temperature with a boundary layer (Figure 5b)	Dirichlet	Variable	Both	Atmosphere conditions on the LS	• Air temperature projections • Conduction from the atmosphere to the LS through a boundary layer	• Current and future air temperatures are known • Thermal conductivity of the boundary layer is constant • Geometry and properties of the boundary layer accurately represent surface processes affecting LS thermal condition	McKenzie et al. (2007)
	Heat exchange boundary layer (Figure 5c)	Cauchy	Variable	Both	LS Water bodies	• Insulation effect of a snow cover • Air temperature projections • Heat conduction and advection from the atmosphere to the LS	• Snow cover properties are known and constant • Other surface thermal processes are not significantly affecting the LS temperature • Energy released by the thawing of the snow (latent heat) does not propagate in the ground • Current and future snow cover depths are known	Dagenais et al. (2020)
	One-way coupling with external surface model (Figure 5d)	Dirichlet or Neumann	Variable	Both	LS Water bodies	• All the surface processes included in the surface model	• Atmospheric, LS and canopy layer conditions are known including future trends • Subsurface conditions do not have any effect on the surface conditions	Kurylyk et al. (2016)
	Two-way coupling with internal equations (Figure 5d)	Built-in function	Variable	Both	LS Water bodies	• Surface processes included in the surface model • Effects of subsurface conditions on surface conditions	• Atmospheric, LS and canopy layer conditions are known including future trends	Jafarov et al. (2018)

Note: The "Used in" column provides one study example for each boundary condition. LS stands for land surface.

conductivity of 1.25 J m^{-1} s^{-1}°C^{-1}. This simplified boundary layer approach (Figure 5b), which has also been used in subsequent studies (e.g., Briggs et al., 2014; Evans & Ge, 2017; McKenzie & Voss, 2013), represents a buffer zone between the atmosphere and the land surface and allows for surface temperatures to be influenced by both the

FIGURE 5 Conceptual model of typical surface thermal boundary condition configurations for cryohydrogeologic models: (a) specified ground-surface temperature (GST); (b) specified air temperature (AT) with a thermal boundary layer (TBL); (c) specified heat flux with a dynamic surface layer (SL); (d) specified temperature or heat flux calculated with a surface energy balance. ET and LH are evapotranspiration and latent heat release by snowmelt, respectively



atmosphere and ground conditions. A very low permeability may be assigned for the thermal boundary layer to allow heat conduction but limit water flow and heat advection in this conceptual buffer zone above the land surface. However, the assigned properties of the "thermal boundary layer" are typically static and do not consider seasonal changes in land surface insulation due to the formation of a snowpack (Zhang, 2005). To simulate the insulating effect of a snowpack, Rushlow et al. (2020) varied the thermal conductivity of the thermal boundary layer to account for snow depth variations. Alternatively, Lamontagne-Hallé et al. (2018) developed a time-dependent heat flux BC that calculates heat conduction through a changing snow cover (Figure 5c). Similarly, Dagenais et al. (2020) used a Cauchy-type BC, built into the model SMOKER, that calculates the natural heat transfer across a dynamic surface layer with spatially and temporally variable properties to represent snow cover in winter and an organic soil layer in summer. Using this BC in the same setting, Albers et al. (2020) found that their numerical model was very sensitive to the near-surface thermal and hydraulic parameters, and to those parameters which define the characteristics of the dynamic surface layer. They thus recommended particular attention be given to characterizing near-surface conditions. To account for more processes and to have a full surface energy balance (Figure 5d), the modeler can also drive the cryohydrogeologic model with an external surface energy model (e.g., Kurylyk et al., 2016).

Assigning BCs in cryohydrogeologic models is a difficult task considering the dynamic impacts of freezing and thawing processes on the model properties. Tables 2 and 3 provide information about different BCs commonly used in modeling studies. BCs that simulate many cold region processes may appear more realistic, but their need for added parameters may also lead to unnecessary complexity and uncertainty (Voss, 2011). Results may indeed match observed field temperature data because there are more calibration parameters to force the desired solution, yet the calibrated parameterization may poorly represent the governing thermal physics, and may lead to increasingly unrealistic future projections (Hill, 2006). We recommend starting with simple BCs and consider developing them into more complex conditions later if necessary. One should also pay attention to the interdependence of the hydraulic and thermal BCs. For example, if specified recharge and specified temperature BCs at the model surface are used, modelers should consider aligning the specified inflowing recharge water temperature with the specified land surface temperature and also consider setting no-flow boundaries when the specified surface temperature drops below 0°C. In the absence of macropores (Mohammed, Kurylyk, Cey, & Hayashi, 2018), which are not well represented in most cryohydrogeologic models, frozen ground has limited infiltration capacity, and forcing recharge into frozen ground may create unrealistic pressure or hydraulic head gradients.

6 | INITIAL CONDITIONS

The initial conditions must be carefully assigned for transient cryohydrogeologic models. The initial temperatures established by the user will be used to generate the initial distribution of liquid water and ice in accordance with the soil-freezing curve, and the distribution of liquid water will be used to generate an initial field of hydraulic and thermal conductivity.

For site-specific models, initial conditions can be based on field data. This approach requires extensive datasets of hydraulic heads, permafrost distributions, and ground temperatures based on geophysical measurements, observation wells, and temperature sensors (e.g., Fortier et al., 2020; Figure 6a). These point measurements can yield interpolated field data to generate the initial (present-day) distribution of temperature and hydraulic head (e.g., Sjöberg et al., 2016). However, gathering such a dataset in an arctic environment can be financially and logistically challenging, and data interpolation may lead to uncertainties and lack of representation due to sporadic data.

For sites that are not data rich, another option is to run a spin-up model to generate the initial conditions for a follow-up transient simulation (e.g., Bense et al., 2012; McKenzie & Voss, 2013). This can be accomplished by driving the spin-up simulation using steady-state BCs (i.e., BC values not varying with time, corresponding to an average of the current pressure or temperature conditions), and stopping the simulation once it has achieved steady-state hydraulic and thermal conditions (Figure 6b). The results from the end of the spin-up simulation can then be used as the initial conditions for a subsequent model run with transient boundary conditions. This approach is often used to form the initial distribution of permafrost in climate warming scenarios (e.g., Bense et al., 2012; Grenier et al., 2013; McKenzie & Voss, 2013) and allows for the model to create its own internally self-consistent initial conditions, assuming that the studied site is initially in equilibrium with the hydroclimatic conditions set as the constant BC. Two steady-state spin-ups, a first for pressure and then a second for temperature, may be necessary to allow for a normal pressure distribution before the ground freezes (e.g., Jafarov et al., 2018; McKenzie & Voss, 2013). If the sub-permafrost aquifer is not being simulated, one could start the spin-up in a fully frozen state instead of an unfrozen one. Karra et al. (2014) found that this approach saves considerable computational time which is highly practical for three-dimensional models.

However, steady-state spin-up simulations may not be the most appropriate approach for all studies, partly due to the assumption that the ground conditions are in equilibrium with the current climate. As Zhang, Chen, and Riseborough (2008) pointed out, permafrost in Canada will continue thawing, even if air temperatures stabilize. Langford et al. (2019) tried two different methods to represent the initial conditions of the discontinuous permafrost at Scotty Creek, Canada: A steady-state run and setting permafrost "blocks" with a uniform temperature. They found that the latter better represented the thermal conditions of their shallow supra-permafrost layer since, at the time of their initial conditions, the simulated permafrost was already out of equilibrium with the climate. However, steady-state simulations may be useful to reproduce past conditions and to start a subsequent spin-up simulation (Figure 6c) that would use long-term time series to create the initial conditions for the simulation of interest.

If seasonality is being considered, which is common in cryohydrogeologic models, we recommend a "dynamic equilibrium spin-up simulation". By assuming constant BCs in the steady-state simulation, several seasonal processes such as the formation of the active layer are not considered. The dynamic equilibrium spin-up simulation (Figure 6c) uses seasonally varying BCs without any yearly changes (i.e., no warming or cooling rate in mean annual conditions). As described in Ge et al. (2011) and Jafarov et al. (2018), such a simulation should be run until no significant difference exists between years. The user can then use the last computed results as initial conditions for the simulation of interest. If long-term air temperature time series are available, they can be used to constrain the model during a spin-up period (e.g., Dagenais et al., 2020). This approach allows the user to create initial conditions for the period of interest that are not necessarily in equilibrium with the current climate, which is more representative of some permafrost systems. As

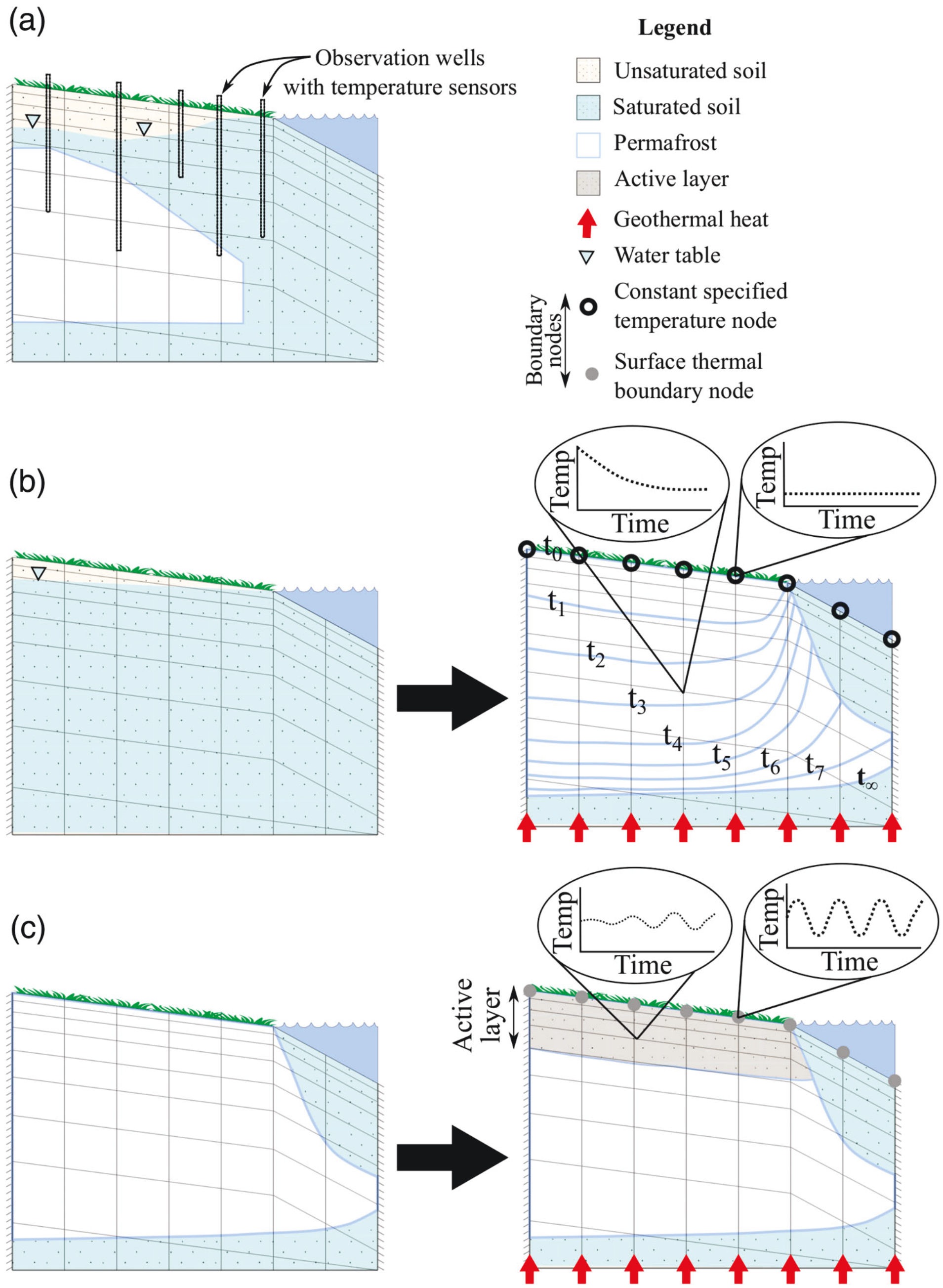


FIGURE 6 Different methods to set the initial conditions for a cryohydrogeologic model using (a) field data, (b) a steady-state spin-up with constant specified temperature nodes, and (c) a dynamic equilibrium spin-up using a seasonally variable surface thermal boundary condition

described in Dagenais et al. (2020), if the spin-up period is long enough, the initial conditions, at least those outside of the permafrost areas, should not adversely affect the modeling results.

7 | TIME STEP SIZE

For transient simulations, the time step size should be carefully addressed. Even if the modeling study does not require results at a fine time scale, it has been shown that a coarse time step size may lead to modeling inaccuracies and instability (Anderson et al., 2015).

A common way to find the appropriate time step is to apply the Courant criterion (Courant, Friedrichs, & Lewy, 1967; Daus et al., 1985):

$$C = \frac{v\,\Delta t}{R\,\Delta x} \leq \frac{P}{2} \tag{2}$$

where C is the Courant number (dimensionless), v is the magnitude of the computed velocity (m s^{-1}), Δt is the time step size (s), Δx is the mesh discretization length (m), and P is the Peclet number (Equation (1)). The thermal retardation (R, dimensionless) represents the assumed instantaneous adsorption of heat by the solid grains of the porous medium and is defined as (Molson et al., 1992):

$$R = \frac{C_o}{\theta S_w \rho_w c_w} \tag{3}$$

where C_o is the bulk heat capacity of the porous media (J $m^{-3\circ}C^{-1}$), θ is the porosity (–), S_w is the water saturation (–), and ρ_w and c_w are the liquid water density (kg m^{-3}) and specific heat capacity (J $kg^{-1\circ}C^{-1}$), respectively. The Courant criterion can be checked with the highest computed velocity in each direction (x, y, and z) after the simulation is complete. Strictly applicable to explicit time-weighting schemes (i.e., terms calculated from the previous time step) for maintaining stability, the Courant criterion nevertheless remains useful for limiting general errors and improving convergence behavior with other schemes.

While respecting the Courant criterion is important, the nonlinearity of the governing equations and boundary condition variability can be limiting factors to determine a suitable time step in cold-regions groundwater modeling. Even if the Courant criterion is satisfied, instability problems caused by a time step that is too large may still occur and should be corrected.

Once the model setup is complete, we recommend a series of short simulations with varying time step sizes to form the basis of comparison. To limit computational time, the largest time step size should be chosen at which no significant difference exists with the outcomes of the simulations using finer time steps. The time step attribution process is similar for cryohydrogeologic models and typical groundwater models. However, particular attention should be given to seasonal, or even daily variations in boundary conditions which may be more impactful in cold regions (Bintanja & van der Linden, 2013). A study should thus choose a time step size that is short enough to represent these processes. One of the findings from the InterFrost project was that many users required a much smaller time step and spatial discretization than initially anticipated in order to match the benchmark problems (Grenier et al., 2018). Some of the cryohydrogeologic modeling tools also use an adaptive time step (ATS, COMSOL, FEFLOW, implementation in FlexPDE, GINETTE, MELT, PermaFOAM, and PFLOTRAN), which will automatically find the optimal time step size based on error estimations and the required temporal accuracy (Diersch, 2014).

8 | CHALLENGES AND RECOMMENDATIONS

The primary objective of this primer is to provide guidelines and suggestions for undertaking cryohydrogeologic modeling. Recent developments have led to increased availability of modeling tools that consider dynamic freezing and thawing processes. So far, the use of these tools to improve our understanding of cold-regions groundwater processes has been primarily for improving our theoretical understanding of cryohydrogeology. Recent studies have been undertaken to apply these tools to real-life settings in highly monitored watersheds (e.g., Dagenais et al., 2020; Evans et al., 2018; Langford et al., 2019). However, despite the importance of understanding the impacts of permafrost thaw at the community scale (White et al., 2007), these models have only rarely been applied for addressing issues related to water resources in the north (e.g., Lemieux, Fortier, Molson, Therrien, & Ouellet, 2020). While guidelines from theoretical modeling may help elucidate the process of setting up and running a cryohydrogeologic model, there are still challenges and limitations that render these tools more difficult to apply in certain settings or applications.

First, many subsurface processes are still not being considered in many cryohydrogeologic models. Cryosuction (i.e., the drawing of water to the freezing front, Schuh et al., 2017), the presence of ice-rich permafrost (Jones, Harrison, Anderson, & Betts, 2018; Walvoord & Kurylyk, 2016) or ice-wedge polygons (Jan et al., 2018; Liljedahl et al., 2016), land subsidence due to permafrost thaw (Painter, Moulton, & Wilson, 2013; Quinton, Hayashi, & Chasmer, 2011), air flow through the porous medium (Wicky & Hauck, 2017), the presence of macro-pores or macro-fractures (Harrington, Mozil, Hayashi, & Bentley, 2018; Mohammed et al., 2018) and effects of salinity on the freezing point (Cochand, Molson, & Lemieux, 2019) are examples of processes or conditions that can influence thermal or hydraulic processes in cold regions. These are potentially important processes, depending on the physical system, that are not fully accounted for in many cryohydrogeologic modeling tools. However, the likelihood that a certain process strongly influences the local hydrology or hydrogeology is dependent on both the scale of the study and the setting in which it occurs. There is also a lack of consideration of surface hydrologic and thermal processes, as evidenced by the overly simplified boundary conditions employed in most studies and by the absence of surface water and energy balance routines in many tools. Before undertaking a cryohydrogeologic modeling study, it is important for the modeler to have a well-developed conceptual model to decide if these complexities should be added. Including processes that could be neglected can significantly increase computational time.

Furthermore, adding more processes or features increases model complexity, therefore increasing the amount of data required, while potentially increasing uncertainty and decreasing the user's understanding of the system. As stated in Voss (2011), a more complex model is not necessarily a more accurate model, as more parameters have to be estimated or calibrated. A case where increased model complexity may help to decrease uncertainties is when the additional complexity allows for the coupling of two co-dependent systems. A good example is the surface energy balance included in some of the aforementioned tools. To increase the accessibility of permafrost heat transfer models outside of the modeling expert community, Fritz et al. (2015) suggested that "Future research should focus on identifying which processes are most important, so that models with varying levels of complexity can be developed for Arctic stakeholders". We propose that the same principle should be applied to cold-regions groundwater models. Our recommendation to modelers is to first focus on identifying the important processes in different environments rather than adding processes to the already complex tools available, and to add varying levels of complexity to their code as suggested by Fritz et al. (2015).

Another challenge for modelers to overcome is making the modeling experience more user-friendly. Most available cryohydrogeologic models do not have a graphical user interface or online support (Table 1), thus increasing the difficulty and the time required to become familiar with a particular code and thereby limiting model applications to a model development team. In many cases, if the user desires additional functions to represent more complex BCs, they must be coded by the user and thus necessitate some knowledge of computer programming. Some codes also offer very little information about sources of error, and do not offer a post-processor to view and analyze the modeling results.

We suggest that developers should focus their efforts not only on code development but also on improving the accessibility of cold-regions groundwater models by (a) developing graphical user interfaces, (b) launching an online support platform where both developers and users can interact and help each other, and (c) creating tutorials to explain the basic components and the important steps to build a cryohydrogeologic model. While in-person workshops are a great initiative to reach new users, they are sometimes expensive to attend and are limited regionally; thus more online training tools would be welcomed. As stated by Bredehoeft (2012), institutional commitment to provide support is key for widely used models, and such institutions should ensure their work is accessible to a wide range of scientists and stakeholders.

In spite of the many areas for advancement in model development and application, much effort has recently been focused on improving the accuracy and utility of cryohydrogeologic models through the addition of more processes and the simplification of the modeling approach for the unfamiliar user. Despite the present limitations, we are confident that these cold-regions groundwater models can enable communities, stakeholders, and scientists from different fields to address fundamental water resources challenges in cold regions. Considering the necessity of including hydrogeology in northern research initiatives (McKenzie et al., 2020), such modeling tools can assist in managing groundwater resources, testing usage scenarios, and developing hydrogeological understanding of cold-regions aquifers.

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CONFLICT OF INTEREST

The authors have declared no conflicts of interest for this article.

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Pierrick Lamontagne-Halle: Conceptualization; visualization; writing-original draft; writing-review and editing. **Jeffrey McKenzie:** Conceptualization; funding acquisition; writing-review and editing. **Barret Kurylyk:** Visualization; writing-review and editing. **John Molson:** Visualization; writing-review and editing. **Laura Lyon:** Writing-review and editing.

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