

Methods Note

Constraining a flow model with field measurements to assess water transit time through a vadose zone

Lamine Boumaiza

Corresponding author: Département des Sciences Appliquées, Université du Québec à Chicoutimi, 555, boulevard de l'Université, Chicoutimi (Québec) Canada G7H 2B1
lamine.boumaiza@uqac.ca

Romain Chesnaux

Département des Sciences Appliquées, Université du Québec à Chicoutimi, 555, boulevard de l'Université, Chicoutimi (Québec) Canada G7H 2B1
Romain_Chesnaux@uqac.ca

Julien Walter

Département des Sciences Appliquées, Université du Québec à Chicoutimi, 555, boulevard de l'Université, Chicoutimi (Québec) Canada G7H 2B1
Julien_Walter@uqac.ca

Christine Stumpp

Institute for Soil Physics and Rural Water Management, University of Natural Resources and Life Sciences, Muthgasse 18, Vienna 1190 Austria
christine.stumpp@boku.ac.at

Conflict of interest: None.

Keywords: SEEP/W, CTRAN/W, water content, hydraulic conductivity, water table.

Article Impact Statement: *Advantage of using comprehensive site measurements for developing an accurate groundwater flow numerical model.*

ABSTRACT

The modeling of thick vadose zones is particularly challenging because of difficulties in collecting a variety of measured sediment properties, which are required for parameterizing the model. Some models rely on synthetic data, whereas others are simplified by running as homogeneous sediment domains and relying on a single set of sediment properties. Few studies have simulated flow processes through a thick vadose zone using real and comprehensive data sets comprising multiple measurements. Here, we develop a flow model for a 7-m-thick vadose zone. This model, combining the numerical codes CTRAN/W with SEEP/W, includes the measured sediment hydraulic properties of the investigated vadose zone and incorporates the actual climate and subsurface conditions of the study site (precipitations, water-table elevations, and stable isotope data). The model is calibrated by fitting the simulated and measured vertical profiles of water content. Our flow model calculates a transit time of one year for the travel of water through the 7-m vadose zone; this estimate matches stable isotope-based results obtained previously for this site. A homogeneous sediment domain flow model, which considers only a single set of sediment properties, produces a transit time that is approximately half the duration of that of the heterogeneous flow model. This difference highlights the importance of assuming heterogeneous material within models of thick vadose zones and testifies to the advantage gained when using real sediment hydraulic properties to parametrize a flow model.

INTRODUCTION

Multiple numerical models have been developed to quantify the basic physical and chemical processes controlling water flow in the vadose zone of aquifers ([Šimůnek and Bradford, 2008](#)). Most studies focus particularly on the shallower part of the vadose zone (depth: 0–2-m), wherein water flow fluctuates greatly due to variability in boundary conditions (precipitation and evapotranspiration) and input, as well as reactive transport processes ([Hopmans and Schoups, 2005](#)). Less attention has been given to water flow within the entire vadose zone often because of a lack of available data for calibrating numerical models. Determining the sediment hydraulic properties for the full profile of relatively thick vadose zones is particularly challenging—especially for establishing the sediment type and texture. Technically, it is difficult and costly to monitor the entire profile of a thick vadose zone ([Hopmans et al., 2002](#); [Konikow, 2011](#); [Vereecken et al., 2016](#); [Vero et al., 2017](#)). Instruments can measure *in situ* the water content and flux rate within the vadose zone ([Brye et al., 1999](#); [Gee et al., 2002](#); [Rimon et al., 2007](#)). Such instrumentation, however, is usually limited to the upper part of the vadose zone or requires the installation of various instruments and drilling ([Rimon et al., 2007](#)).

Integrating the heterogeneity of sediment properties across a thick vadose zone represents another challenge for the accurate modeling of water movement within this zone; this is particularly true when the vadose zone is very heterogeneous. For this reason, most studies of the vadose zone do not consider the variability of hydraulic properties and thus assume a homogeneous vadose zone characterized by a single set of effective hydraulic properties ([Corwin et al., 2006](#); [Szymkiewicz et al., 2018](#)). Nonetheless, actual profiles of sediment hydraulic properties through the vadose zone are highly non-uniform and vary

greatly with depth (Potrykus et al., 2018). Sediment texture information (e.g., gravel, sand, clay, silt) can be combined with pedotransfer functions (pedotransfer functions are predictive functions of soil properties based on other known measured soil properties such as soil texture) to estimate hydraulic properties. However these estimates can be uncertain, and occasionally differ from the true values of hydraulic properties, if the sediment texture information introduced into the numerical model is not sufficiently representative of the actual sediment texture (Durner, 1994; Holt and Nicholl, 2004). Uncertainties stemming from unrealistic sediment properties that are introduced into the numerical model may greatly affect the accuracy of the estimated water transit-time through the vadose zone (Mattern and Vanclooster 2010). Consequently, using sufficiently accurate information on the measured sediment properties and the sediment grain-size distribution is expected to reduce uncertainties when the pedotransfer functions are employed. Mattern and Vanclooster (2010) used a physically based conceptual model (HYDRUS 1D) to estimate water transit time through the vadose zone. Due to the limited available information of the site's sediment hydraulic properties, they combined three generic approaches to estimate these properties required for parameterizing their model: 1) the HYDRUS catalog (Carsel and Parrish, 1988), 2) Rosetta (Schaap et al., 2001), 3) and the existing literature related to measured hydraulic properties (Hupet et al., 2004; Javaux and Vanclooster, 2006, 2004). Nonetheless, the uncertainties stemming from the unrealistic sediment properties introduced into the HYDRUS 1D model greatly affected estimates of water transit time through the vadose zone. Recently, oxygen and hydrogen stable isotopes in pore water have been used to estimate sediment hydraulic properties (e.g., Groh et al., 2018; Mattei et al., 2020; Sprenger et al., 2015). Pore water stable

isotopes also provide valuable insight into the infiltration process (Chesnaux and Stumpp, 2018; Thomas et al., 2013), and this information can derive transit times across the vadose zone (Stumpp et al., 2009).

Studies of the profiles of relatively thick vadose zones include 0–6-m depth profiles in glacial till (Stumpp and Hendry, 2012), 0–4-m depth profiles in loess soils (Sprenger et al., 2016), and 0–7-m depth profiles in sandy sediments (Boumaiza et al., 2020). Direct sampling of deep vadose zones requires laborious drilling. The recovery of other complementary data (e.g., precipitation, groundwater recharge, water table level), which help constrain flow models of thick vadose zones, is also challenging (Groh et al., 2016; Heidbüchel et al., 2013; Levitt et al., 2005). Due to these constraints, few studies have compiled and applied comprehensive data sets of diverse measurements from relatively thick vadose zones (e.g., Mohanty et al., 2002; Western and Grayson, 1998). The laborious collection of such data sets is, therefore, one of the most valuable tasks in modeling studies of the vadose zone.

This study follows a comprehensive technical framework to develop a flow model that is based on information obtained from the sampling of a thick vadose zone using high-resolution sediment cores. This model investigates a 7-m-thick heterogeneous vadose zone in the Saint-Honoré aquifer, located in the Saguenay–Lac-St-Jean region of Quebec (Canada). This model (i) considers the measured sediment hydraulic properties, which are estimated from the sediments collected throughout the vadose zone, (ii) is constrained by the use of actual climate and subsurface data (precipitation, water-table level, and stable isotope data), and (iii) is calibrated by fitting the simulated and measured vertical water-content profiles. We evaluate the model outcome by comparing the simulated water

transit time with that obtained for the same site using a stable isotope–based approach. We highlight the importance of incorporating the observed vertical heterogeneous sediment properties through the vadose zone by comparing the results with those obtained when only considering a single set of effective sediment properties for the entire vadose zone (homogeneous domain).

METHODS AND MATERIALS

Fieldwork and laboratory analyses

Subsurface sediment sampling

We selected the Saint-Honoré aquifer because the thickness of the vadose zone of this aquifer is up to 7 m, and there is relevant available information related to the site, including groundwater recharge and water-table elevations (Boumaiza, 2008; Boumaiza et al., 2020, 2019b; Chesnaux and Stumpp, 2018; Labrecque et al., 2020; Tremblay, 2005). A borehole was drilled on 23 May 2019 using a hand threshing-beating auger. Continuous sediment cores were subsequently collected from a split-spoon sampler (0.69-m-long, 0.05-m-diameter), and we subsampled at an average interval of 12 cm. The split-spoon was cleaned using dry towels after the collection of each sediment sample to minimize water transmission between sediment samples during the continuous drilling. Following an *in situ* visual description (sediment texture, color, humidity) of the collected sediment samples, the samples were immediately stored in separately labeled polyethylene Ziploc[®] bags and tightly sealed to prevent moisture loss due to evaporation. A total of 58 sediment samples were collected and sent to the laboratory.

Sediment properties determined by drying

In the laboratory, we placed a subset of each sediment sample into individual metal cylinders of known mass and volume. We weighed each sample and then dried the samples in an oven for 48 hours at a temperature of 105 °C. We then weighed the dried samples (in g) and determined the total wet and dry sediment mass (in g). First, the gravimetric water content (GWC) of each single representative sediment subsample, expressed in %, was determined according to Eqn. 1 (Gardner, 1965). Afterwards, the dry bulk density (D_b), expressed in g/cm³, was determined using Eqn. 2 (Black et al., 1965). Once D_b was known, the volumetric water content (VWC), expressed in %, was calculated for each sediment sample using Eqn. 3 (Gardner, 1965) assuming a water density (ρ_w) of 1 g/cm³. Porosity (n), expressed in %, was calculated using Eqn. 4 (Black et al., 1965) assuming a particle density (ρ_p) of 2.69 g/cm³ (Boumaiza et al., 2015). The void ratio (e) was calculated using Eqn. 5. The parameters n and e were further used to estimate the saturated hydraulic conductivity (K_s) (Table 1).

$$\text{GWC} = \frac{\text{weight of wet soil} - \text{weight of dry soil}}{\text{weight of dry soil}} \cdot 100 \quad (1)$$

$$D_b = \frac{\text{weight of dry soil}}{\text{volume of specific cylinder}} \quad (2)$$

$$\text{VWC} = \theta_G \cdot (D_b / \rho_w) \quad (3)$$

$$n = 100 \cdot \left[1 - \left(\frac{D_b}{\rho_p} \right) \right] \quad (4)$$

$$e = \frac{n}{1 - n} \quad (5)$$

Sediment properties determined by sieve grain-size analysis

To have a sufficient quantity of sediment for grain-size sieve analyses, we grouped successive sediment samples—collected from the drilled borehole—according to their visual similarity in terms of sediment texture and structure. We used Wentworth’s classification ([Wentworth, 1922](#)) for reporting grain sizes (clay: <0.003 mm; silt: 0.003–0.06 mm; sand: 0.06–2 mm, gravel: 2–64 mm). We used the obtained grain-size classes to predict K_s via five empirical models: [Hazen \(1892\)](#), [Beyer \(1964\)](#), [Chapuis \(2004\)](#), [Sauerbrey \(1932\)](#), and USBR ([Vukovic and Soro, 1992](#)). Given the different limitations of each these empirical equations, as presented in Table 1, some equations may not be applicable to certain sediment samples. Thus, a K_s value was calculated for each sediment sample by using only the applicable empirical equations. A single average K_s value was then calculated, for each sediment sample, representing the geometric mean value as it was approved to provide a reliable mean approximation of a set of K_s values ([Zappa et al., 2006](#)). [Table 1](#) summarizes the applied empirical equations for calculating K_s and their limitations in their application.

Table 1. Selected empirical methods used to predict K_s and the conditions required for their application.

| Method | Empirical formula | Conditions |
|-----------|---|--|
| Hazen | $K_s \text{ (cm/s)} = (d_{10})^2$ with d_{10} in mm | a. Sand and gravel b. $C_u \leq 5$ c. $0.1 \text{ mm} \leq d_{10} \leq 3 \text{ mm}$ |
| Chapuis | $K_s \text{ (cm/s)} = 2.4622((d_{10})^2 e^3)/(1 + e)^{0.7825}$ with d_{10} in mm | a. All natural soils without plasticity b. $0.003 \text{ mm} \leq d_{10} \leq 3 \text{ mm}$ c. $0.3 \leq e \leq 1$ |
| Beyer | $K_s \text{ (cm/s)} = 0.45 (d_{10})^2 \log (500/C_u)$ with d_{10} in mm | a. Sand b. $0.06 \text{ mm} \leq d_{10} \leq 0.6 \text{ mm}$ c. $1 \leq C_u \leq 20$ |
| Sauerbrey | $K_s \text{ (cm/s)} = 2.436n^3 (d_{17})^2/(1 - n)^2$ with d_{17} in mm | a. Sand and silty sand b. $d_{10} \leq 0.5 \text{ mm}$ |
| USBR | $K_s \text{ (cm/s)} = 0.36 (d_{20})^{2.3}$ with d_{20} in mm | a. Sand and gravel b. $C_u \leq 5$ |

d_x : effective grain size of x (% by weight of soil)

C_u : coefficient of uniformity for non-plastic soils ($C_u = d_{10}/d_{60}$)

General description of the used numerical codes

GeoStudio software contains several codes, including the codes SEEP/W and CTRAN/W (Geo-Slope, 2019) that are used in this study. Numerous studies have assessed the robustness of these codes (Chapuis et al., 2001; Chapuis and Aubertin, 2001; Chapuis and Chenaf, 2003; Chesnaux and Allen, 2008; Eltarabily and Negm, 2015). SEEP/W is a finite element code used to solve one- to three-dimensional problems either under a transient or steady-state groundwater flow regime for both saturated and

saturated/unsaturated conditions. This code solves numerically Darcy's law equation (Eqn. 6; Darcy 1856) that is combined to the principle of fluid mass conservation, expressed by the Richards equation (Eqn. 7; Richards 1931). In Eqn. 6, v is the Darcian velocity [LT^{-1}], K is the hydraulic conductivity [LT^{-1}], and ∇h is the head gradient [-]. In Eqn. 7 Q is the sink or source term [T^{-1}], θ is volumetric water content [-], and t is time [T].

$$v = -K \nabla(h) \quad (6)$$

$$-div(v) + Q = \frac{\partial \theta}{\partial t} \quad (7)$$

SEEP/W considers the sediment characteristic functions $K(u)$ and $\theta(u)$, in which (u) is the pore water pressure, $K(u)$ is the hydraulic conductivity function, and $\theta(u)$ is the VWC function. The code solves for the relation between $\theta(u)$ and (u) and that between $K(u)$ and (u). Both $\theta(u)$ and $K(u)$ may be determined in the laboratory using various direct and indirect measurement methods (e.g., Klute, 1986; Fredlund and Rahardjo, 1993; Marshall *et al.*, 1996). Otherwise, $\theta(u)$ and $K(u)$ may also be predicted respectively from a grain-size distribution curve (e.g., Fredlund and Xing, 1994; Barbour, 1998; Aubertin *et al.*, 2003) and the VWC function, calculated by various methods (e.g., Green and Corey, 1971; Van Genuchten, 1980; Fredlund *et al.*, 1994). CTRAN/W is a finite element code that can be used to simulate solute transport in the porous media. CTRAN/W is combined with SEEP/W, where the latter first solves water flow, which is a prerequisite step for solving solute transport using CTRAN/W. Solute transport can be simulated as purely advective transport using a particle-tracking function, where the fluid is represented by particles that move in porous media in proportion with the water flow velocity. The

particle-tracking function allows for tracking the groundwater flow pathways and calculating the particles' tracking time (Geo-Slope, 2019).

Numerical flow model implementation

Using SEEP/W, we modeled the investigated vadose zone as a 1-D vertical column. The column abscissa x , representing the width of the vadose zone, is limited to 1 m as the modeling is undertaken in 1-D. The ordinate y , representing the depth of the vadose zone, is maintained at 7 m, as drilled in the field. The heterogeneity of the vadose zone is simulated via a model divided into several layers. The column model domain is divided into 58 layers, each 0.12-m thick, reflecting the average interval of sediment sampling. This model has a final 0.04-m-thick layer added to the bottom to attain a profile depth of exactly 7 m.

Each layer of the domain is considered to be independent, as specified by its unique sediment properties. Each sediment layer is first constrained by its measured sediment porosity and its measured effective grain sizes d_{10} and d_{60} (Table 2). Introducing these data produces a curve that defines the relationship between VWC and pressure throughout the sediment layer, including the residual water content, which is determined at the highest pressure. This information is then combined with the saturated hydraulic conductivity of the sediment layer (Table 2) to define the unsaturated hydraulic conductivity distribution as a function of pressure. This step is done using the pedotransfer function of Fredlund *et al.* (1994) integrated into SEEP/W. The column model domain, including the 58 layers, is discretized into 0.01-m² meshing square elements, thereby involving a total of 70 000 elements in the domain and having 70 801 nodes.

Flow model processing is performed in three main phases: (1) basic equilibrium modeling assuming no-flow conditions; (2) simulation of transient water flow conditions under one-year spin-up period to determine the simulated VWC distribution as a function of depth; and (3) running of the one-year transient conditions for a calibrated flow model. The calibration process involves adjusting the sediment porosity and saturated hydraulic conductivity for all of the model's layers until the numerical VWC profile agrees with the measured profile. For the boundary conditions, the sides of the model's vertical column are always assigned without any specification, meaning they are considered to be impermeable borders. For the basic equilibrium flow model, a zero-flux upper boundary and a zero-pressure-head lower boundary are applied. During the transient spin-up period, the upper boundary condition is modified to a transient daily water cubic flux. The time frame for the actual simulation period is selected based on a mean water transit time determined using the previous results over one year through the investigated vadose zone (Boumaiza et al., 2020). Once the SEEP/W vadose-zone flow model is calibrated, the CTRAN/W code is then used by introducing a particle at the top of the flow model. The forward particle-tracking option of the CTRAN/W code produces the pathway and tracking time for the introduced particle. To investigate whether sediment heterogeneity is crucial to the model when describing water flow within the vadose zone, we ran a second flow model characterized by homogenized hydraulic properties. The abovementioned steps are then repeated, although this second run uses a homogeneous domain. This domain is defined by a single set of values for sediment properties, which are weighted as the average of the measured values.

Determining boundary conditions of the vadose zone

Lower boundary condition

Flow conditions in the vadose zone can be affected by the height of the water table (lower model boundary condition), which varies over time. Therefore, long-term monitoring of fluctuations of the water table at the study site are required. We relied on the water-table data of [Labrecque *et al.* \(2020\)](#), collected from piezometer PZ-1, which is located about 100 m from the borehole drilled in this study. This piezometer, which is equipped with a pressure sensor to monitor the local fluctuations of the water table, provided representative water table levels under local natural flow conditions—the site is not affected by any pumping well. Although the year of daily data recorded by [Labrecque *et al.* \(2020\)](#) (9 November 2016 to 9 November 2017) does not cover the year immediately prior to sediment sampling day (22 May 2019), we nonetheless regard this data set as representative for yearly fluctuations in the local water table. The error associated with using the water-table data of [Labrecque *et al.* \(2020\)](#) should be minimal because seasonal climate characteristics have not experienced any significant changes over the last years. We also estimated the maximum height of the subsurface sediment capillary fringe (h_c expressed in mm), in which groundwater rises up from a water table by capillary action to fill sediment pores, using [Eqn. 8 \(Lane and Washburn, 1946\)](#).

$$h_c = -900 \ln(d_{10}) - 1540 \quad (8)$$

Upper boundary condition

The upper model boundary condition is assumed to be affected by precipitation, limited to that captured within the year before sediment sampling day (22 May 2019). We selected a one-year data window on the basis of the water transit time through the investigated vadose zone (one year), as determined by stable isotope-based approach (Boumaiza et al., 2020). In the present study, we considered as much as possible the actual variation over time of the precipitation, over the considered year of interest, in order to more accurately represent the upper boundary conditions. All daily precipitation data were obtained from the Bagotville climate station, located 25 km from the Saint-Honoré aquifer (Government of Canada, 2019). Precipitation represents all rainfall and/or snowmelt converted into a water equivalent. We used a 10:1 ratio for this conversion; therefore, 1 cm of snow on the ground was equal to 1 mm of liquid precipitation (Potter, 1965). As in Boumaiza et al. (2020), we converted the total snowfall during winter into a water equivalent and then distributed this precipitation equally over the spring period (after 6 April 2019), and this converted water amount is then added to the daily rainfall captured over the spring season when relevant. The limited amount of snow that fell during spring 2019 was converted on a daily basis and then combined with daily rainfall recorded for the season.

RESULTS AND DISCUSSION

Sediment properties

Volumetric water content

The upper part of the vertical VWC profile through the investigated vadose zone, 0 to 50 cm below the ground surface (b.g.s.), presented elevated values of VWC (Figure 1).

These high values corresponded to recently infiltrated snowmelt, as the borehole was drilled in the spring (May 2019). As expected, VWC showed a marked vertical variation, which related to different infiltration events that slowly flowed through the vadose zone, rather than reflecting any influence of variable sediment texture of the aquifer. The VWC profile showed less variation from 50 to 300 cm relative to that between 300 and 700 cm. This reduced variation from 50 to 300 cm related to less water infiltration over a given period or a reaching of equilibrium conditions. This depth corresponded to water originating from the period before melting (winter), when the frozen soil surface acted as a barrier to water infiltration. The variability in VWC over the deeper interval—from 300 to 700 cm—reflected various water percolation scenarios, which were potentially related to precipitation events having occurred before winter, a season known to be rainy in humid Nordic regions (Boumaiza et al., 2020; Chesnaux and Stumpp, 2018).

Saturated hydraulic conductivity

Considering Wentworth’s classification (Wentworth, 1922) used in the present study, the sediment grain-size distribution in Figure 2 shows that samples were dominated by sand, albeit with various sand fractions in the individual depth segments (Figure 3) indicating some vertical sediment heterogeneity. Using the measured sediment properties n and e combined with the effective grain-size characteristics (Table 2)—obtained using the grain-size curves (Figure 2)—we calculated an average K_s value for each depth interval (the cumulative total of selected successive sediment subsamples is indicated as a “grouped subsample” in Table 2) using the five empirical methods described in Table 1. The average calculated K_s values ranged from 4.4×10^{-2} to 9.1×10^{-2} cm/s (Table 2) due to the vertical various sand fractions combined with the variability of physical properties

of the sediment (Table 2); they corresponded to the expected values for the Saint-Honoré granular aquifer (Boumaiza, 2008; Boumaiza et al., 2019b, 2017).

Table 2. Sediment characteristics as obtained from grain-size curves and sediment-drying analyses.

| Sample ID* | Grouped subsamples | Depth interval b.g.s. (cm) | d_{10} (mm) | d_{17} (mm) | d_{20} (mm) | d_{50} (mm) | d_{60} (mm) | C_u (-) | n (-) | e (-) | Average K_s (cm/s) |
|------------|--------------------|----------------------------|---------------|---------------|---------------|---------------|---------------|-----------|---------|---------|----------------------|
| A | 1 to 2 | 00.00–20.32 | 0.20 | 0.27 | 0.30 | 0.65 | 0.80 | 4.00 | 0.79 | 3.76 | 9.1E-02 |
| B | 3 to 4 | 20.32–42.67 | 0.18 | 0.24 | 0.27 | 0.52 | 0.68 | 3.78 | 0.61 | 1.56 | 4.4E-02 |
| C | 5 to 11 | 42.67–152.4 | 0.25 | 0.31 | 0.36 | 0.75 | 0.90 | 3.60 | 0.49 | 0.96 | 7.3E-02 |
| D | 12 to 16 | 152.4–213.35 | 0.28 | 0.35 | 0.39 | 0.76 | 0.88 | 3.14 | 0.47 | 0.89 | 8.4E-02 |
| E | 17 to 22 | 213.35–294.63 | 0.25 | 0.32 | 0.37 | 0.80 | 0.95 | 3.80 | 0.43 | 0.75 | 6.0E-02 |
| F | 23 to 28 | 294.63–359.65 | 0.27 | 0.33 | 0.38 | 1.00 | 1.40 | 5.19 | 0.43 | 0.75 | 7.6E-02 |
| G | 29 to 37 | 359.65–467.33 | 0.20 | 0.28 | 0.34 | 0.90 | 1.15 | 5.75 | 0.43 | 0.75 | 4.8E-02 |
| H | 38 to 47 | 467.33–579.08 | 0.28 | 0.31 | 0.35 | 0.60 | 0.71 | 2.54 | 0.46 | 0.85 | 7.4E-02 |
| I | 48 to 58 | 579.08–700 | 0.25 | 0.28 | 0.30 | 0.49 | 0.55 | 2.20 | 0.46 | 0.85 | 5.9E-02 |

*Example: Sample D represents the five sediment subsamples 12 to 16 collected successively from 152.4 cm to 213.35 cm b.g.s.

Lower and upper boundary conditions

Over the monitored year in Figure 4, the water table fluctuated between 156.14 and 157.18 m, a range of 1.04 m. These water-table fluctuations reflect the change in weather conditions of the study area, which is characterized by short, hot, and humid summers, cold and snowy winters, and rainy springs and autumns. We observed the highest elevation, 157.18 m, on day 225 (i.e., 23 June 2017) during the post-snowmelt period. If we assume an average d_{10} of 0.2 mm in Eqn. 8, we obtain a maximum height of the sediment capillary rise of 5.30 cm. Accordingly, the highest water table was estimated at

157.23 m (157.18 m + 0.053 m). Comparing this height of the water table (157.23 m) to that of the ground surface at the borehole site (164.44 m), we calculated a vadose zone of 7.21 m. As the flow model was limited to a depth of 7 m, we could assume that the water-table fluctuations did not affect the investigated vadose zone. The lower boundary of the flow model was therefore considered as representing a free water boundary condition.

We estimated groundwater recharge rates of 71% and 63% for the Saint-Honoré aquifer for winter/spring and summer/autumn, respectively (Boumaiza et al., 2020, 2019a). For winter/spring, the 71% groundwater recharge rate represented the effective amount of water that infiltrated into the aquifer, i.e., only 71% of the precipitation captured during this period entered the aquifer. Therefore, we assume that for winter/spring (from 10 November 2018 to 22 May 2019), the daily infiltrating water flux was therefore 71% of the daily captured precipitation. For example, the daily captured precipitation for 22 May 2019 was 4.7 mm, which converts to an initial daily cubic flux of $5.44 \times 10^{-8} \text{ m}^3/\text{s}$. However, relying on the 71% infiltration rate, we then calculated the true daily infiltrating water cubic flux at $3.86 \times 10^{-8} \text{ m}^3/\text{s}$ as the amount of precipitation entering the aquifer. We applied this adjustment to each daily infiltrating water flux over the winter/spring. We then used the same adjustment calculations for summer/autumn (21 May to 9 November 2018), using a groundwater recharge rate of 63%. The transient daily cubic-flux values (m^3/s) over the year (Figure 5) also included zero unit flux values, which corresponded to the period where the snowpack and a frozen soil surface acted as barriers to water infiltration. Our flow model was constrained by this calculated transient upper boundary water flux.

Flow model simulations and validation

The simulated VWC profile, related to the calibrated flow model having a heterogeneous domain, agreed well with the measured VWC profile (Figure 6). This profile matched the measured VWC profile to a much higher degree than did the profile based on a homogeneous domain. We can identify two advantages for determining the specific heterogeneous properties of a vadose zone. First, our chosen calibration process allowed the simulated VWC profile to fit well with the measured profile. If the measured vertical VWC profile is unknown or unavailable, this form of calibration cannot occur. The second advantage relates to our calibration approach. Given the significant variations within the measured vertical VWC profile (Figure 1), it is difficult to obtain a good fit between the simulated and measured VWC profiles when the vadose zone is simulated by a single set of sediment properties (homogeneous domain). For the flow model of 58 layers, however, the calibrating process involves adjusting (changing) sediment porosity and saturated hydraulic conductivity across all of the model's layers until the numerical VWC profile agrees with the measured profile. This approach offers the advantage of making smaller-scale adjustments of sediment properties within an independent layer—in cases where the simulated and measured VWC profiles do not agree—and improves the fit between the simulated and measured vertical VWC profiles.

We did not observe a less permeable material (e.g., clay) in the vadose zone, which could act as a perched barrier to vertical water flow. Therefore, particle transport was simulated as a purely advective transport that assumes only a vertical downward water flow from the ground surface to the water table. We did not include dispersive transport because the complete vadose zone was dominated by sandy material in which the intensity of

preferential pathways, which contributes to multiple flows, was expected to be lower. We calculated the transit times of introduced particles to verify the corresponding tracking depth–distance through the vadose zone. We tracked the particle pathway for a series of transit times. After 0.36 years ([Figure 7a](#)), 0.72 years ([Figure 7b](#)), 0.88 years ([Figure 7c](#)), and 1 year ([Figure 7d](#)), we observed a corresponding depth–distance of 2.34 m, 5.22 m, 6.72 m, and 7 m, respectively. [Boumaiza et al. \(2020\)](#), using a stable isotope–based approach, obtained a one-year transit time for the same vadose zone; this duration agreed with our numerical modeling–based estimate. Therefore, our proposed technical framework provided reasonable results. Future studies would benefit from examining variable snowmelt fluxes, as upper model boundary conditions, not only to investigate the average water transit-time through a thick vadose zone, but also to investigate the variability over time of water transit-time.

To illustrate the benefits of considering a material’s heterogeneity in modeling the vadose zone, we assessed the water transit time through a flow model with an effective homogeneous domain. In this case, we estimated that the particle travels through the 7-m homogeneous vadose zone in 0.44 years, roughly half the time estimated by the heterogeneous sediment domain flow model and stable isotopes. Hence, the observed variability of the hydraulic properties of the sediment through the vadose zone is required to be considered in such vadose zone investigations, rather than assuming a homogeneous domain with uniform hydraulic properties. Most studies of the vadose zone assume a homogeneous vadose zone characterized by a single set of effective hydraulic properties ([Corwin et al., 2006](#)). This study has confirmed that the uncertainties stemming from such assumptions have greatly affected the outcomes.

CONCLUSION

Our numerical vadose zone flow model 1) includes the observed heterogeneity of materials comprising the 7-m-thick vadose zone; 2) is constrained by climate and subsurface conditions (precipitation dominated by snowmelt, water-table fluctuations, and stable isotope data) observed in the field; and 3) is calibrated by fitting the simulated vertical VWC profiles to a measured profile. This flow model estimates a one-year transit time for water through the 7-m-thick vadose zone, an estimate that agrees with previous stable isotope-based estimates for the same site. This agreement occurs only when the vadose zone is considered as heterogeneous, and sediment properties are assigned to individual depth intervals. A flow model that assumes homogeneous sediment through the vadose zone, thus relying on a single set of sediment properties, produces an erroneous transit time. Our study therefore illustrates the advantage of using comprehensive data sets, to develop accurate flow models for thick vadose zones, including stable isotope data. The upper model boundary condition is constrained by precipitation, limited to one year before the sediment sampling day, on the basis of the water transit-time previously determined by the stable isotope-based approach. Moreover, the water transit-time assessed in the present study was validated with that previously assessed by using the stable isotope-based approach. This study also highlights the advantages of applying a measured VWC profile to the model calibration process. The vadose zone model was calibrated in the present study by fitting the simulated vertical VWC profile to the measured profile. Hence, this calibrated model could be efficiently employed to investigate other scenarios, by applying other, different upper and lower boundary conditions, reflecting other climate conditions. The technical

framework used in this study offers a tool with which practitioners using numerical modeling can identify and obtain the relevant data for developing an accurate model to estimate transit times of water through the vadose zone.

ACKNOWLEDGMENTS

The authors would like to thank the Natural Sciences and Engineering Research Council of Canada (Discovery grant held by Prof. Romain Chesnaux) for funding this project. David Noël is thanked for his help with the core sediment sampling at the Saint-Honoré aquifer (Saguenay, Quebec). Ms. Josée Kaufmann is thanked for editorial collaboration.

REFERENCES

- Aubertin, M., Mbonimpa, M., Bussière, B., Chapuis, R.P., 2003. A model to predict the water retention curve from basic geotechnical properties. *Canadian Geotechnical Journal* 40, 1104–1122.
- Barbour, S.L., 1998. Nineteenth Canadian Geotechnical Colloquium: The soil-water characteristic curve: a historical perspective. *Canadian Geotechnical Journal* 35, 873–894.
- Beyer, W., 1964. Zur bestimmung der wasserdurchlässigkeit von kiesen und sanden aus der kornverteilungskurve [On determining the water permeability of gravel and sand from the grain distribution curve]. *Wasserwirtsch Wassertech* 14, 165–168.
- Black, C.A., Evans, D.D., White, J.L., Ensming, L.E., Clark, F.E., Dinaueu, R.C., 1965. *Methods of soil analysis, Part 1, Physical and mineralogical properties including staistics of measurement and sampling*. American Society Agronomy, Inc Publisher. Madison. Wisconsin USA.

- Boumaiza, L., 2008. Caractérisation hydrogéologique des hydrofaciès dans le paléodelta de la rivière Valin au Saguenay [Hydrogeological characterization of hydrofacies in the Valin River Paleodelta in Saguenay]. Master's Thesis, Université du Québec à Chicoutimi, Québec, Canada.
- Boumaiza, L., Chesnaux, R., Stumpp, C., 2019a. Assessing groundwater recharge and evapotranspiration in Nordic humid region dominated by snowmelt, in: The International Association of Hydrogeologists Conference, Malaga, Spain.
- Boumaiza, L., Chesnaux, R., Walter, J., Stumpp, C., 2020. Assessing groundwater recharge and transpiration in a humid northern region dominated by snowmelt using vadose-zone depth profiles. *Hydrogeology Journal* 28, 2315–2329.
- Boumaiza, L., Rouleau, A., Cousineau, P.A., 2019b. Combining shallow hydrogeological characterization with borehole data for determining hydrofacies in the Valin River paleodelta, in: Proceedings of the 72nd Canadian Geotechnical Conference, St-John's, Newfoundland, Canada. p. 8.
- Boumaiza, L., Rouleau, A., Cousineau, P.A., 2017. Determining hydrofacies in granular deposits of the Valin River paleodelta in the Saguenay region of Quebec, in: Proceedings of the 70th Canadian Geotechnical Conference and the 12th Joint CGS/IAH-CNC Groundwater Conference, Ottawa, Ontario, Canada. p. 8.
- Boumaiza, L., Rouleau, A., Cousineau, P.A., 2015. Estimation de la conductivité hydraulique et de la porosité des lithofaciès identifiés dans les dépôts granulaires du paléodelta de la rivière Valin dans la région du Saguenay au Québec, in: Proceedings of the 68th Canadian Geotechnical Conference, Quebec City, Quebec, Canada. p. 9.

- Brye, K.R., Norman, J.M., Bundy, L.G., Gower, S.T., 1999. An Equilibrium Tension Lysimeter for Measuring Drainage through Soil. *Soil Science Society of America Journal* 63, 536–543.
- Carsel, R.F., Parrish, R.S., 1988. Developing joint probability distributions of soil water retention characteristics. *Water Resources Research* 24, 755–769.
- Chapuis, R.P., 2004. Predicting the saturated hydraulic conductivity of sand and gravel using effective diameter and void ratio. *Canadian Geotechnical Journal* 41, 787–795.
- Chapuis, R.P., Aubertin, M., 2001. A simplified method to estimate saturated and unsaturated seepage through dikes under steady-state conditions. *Canadian Geotechnical Journal* 38, 1321–1328.
- Chapuis, R.P., Chenaf, D., 2003. Variable-head field permeability tests in driven flush-joint casings: Physical and numerical modeling. *Geotechnical Testing Journal* 26, 245–256.
- Chapuis, R.P., Chenaf, D., Bussi re, B., Aubertin, M., Crespo, R., 2001. A user’s approach to assess numerical codes for saturated and unsaturated seepage conditions. *Canadian Geotechnical Journal* 38, 1113–1126.
- Chesnaux, R., Allen, D.M., 2008. Simulating nitrate leaching profiles in a highly permeable vadose zone. *Environmental Modeling and Assessment* 13, 527–539.
- Chesnaux, R., Stumpp, C., 2018. Advantages and challenges of using soil water isotopes to assess groundwater recharge dominated by snowmelt at a field study located in Canada. *Hydrological Sciences Journal* 63, 679–695.
- Corwin, D.L., Hopmans, J., De-Rooij, G.H., 2006. From Field- to Landscape-Scale Vadose Zone Processes: Scale Issues, Modeling, and Monitoring. *Vadose Zone*

Journal 5, 129–139.

Darcy, H., 1856. Les fontaines publiques de la ville de Dijon. Victor Dalmont, Paris.

Durner, W., 1994. Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research* 30, 211–223.

Eltarabily, M.G.A., Negm, A.M., 2015. Numerical Simulation of Fertilizers Movement in Sand and Controlling Transport Process via Vertical Barriers. *International Journal of Environmental Science and Development* 6, 559–565.

Fredlund, D.G., Rahardjo, H., 1993. *Soil Mechanics for Unsaturated Soils, Soil Mechanics for Unsaturated Soils*. John Wiley and Sons, Inc., New York.

Fredlund, D.G., Xing, A., 1994. Equations for the soil-water characteristic curve. *Canadian Geotechnical Journal* 31, 521–532.

Fredlund, D.G., Xing, A., Huang, H., 1994. Predicting the permeability function for unsaturated soils using the soil-water characteristic curve. *Canadian Geotechnical Journal* 31, 533–546.

Gardner, W.H., 1965. Water content. In: Black, C.A. (Ed.), *Methods of Soil Analysis*. American Society of Agronomy, Inc., Madison, Wisconsin, USA 82–127.

Gee, G.W., Ward, A.L., Caldwell, T.G., Ritter, J.C., 2002. A vadose zone water fluxmeter with divergence control. *Water Resources Research* 38, 1–7.

Geo-Slope, 2019. Seepage modeling with SEEP/W. Geo-Slope International Ltd.

Government of Canada, 2019. Canada's national climate archive.

http://www.climate.weatheroffice.ec.gc.ca/climate_normals/ [consulted in July 2019].

Green, R.E., Corey, J.C., 1971. Calculation of hydraulic conductivity. A further

- evaluation of some predictive methods. *Soil Sci Soc Amer Proc* 35, 3–8.
- Groh, J., Stumpp, C., Lücke, A., Pütz, T., Vanderborght, J., Vereecken, H., 2018. Inverse Estimation of Soil Hydraulic and Transport Parameters of Layered Soils from Water Stable Isotope and Lysimeter Data. *Vadose Zone Journal* 17, 170168.
- Groh, J., Vanderborght, J., Pütz, T., Vereecken, H., 2016. How to Control the Lysimeter Bottom Boundary to Investigate the Effect of Climate Change on Soil Processes? *Vadose Zone Journal* 15.
- Hazen, A., 1892. Some physical properties of sand and gravel, with their special reference to their use in filtration. 24th annual report, Boston, Massachusetts State Board of Health 34, 539–556.
- Heidbüchel, I., Troch, P.A., Lyon, S.W., 2013. Separating physical and meteorological controls of variable transit times in zero-order catchments. *Water Resources Research* 49, 7644–7657.
- Holt, R.M., Nicholl, M.J., 2004. Uncertainty in Vadose Zone Flow and Transport Prediction. *Vadose Zone Journal* 3, 480–484.
- Hopmans, J., Schoups, G., 2005. Soil Water Flow at Different Spatial Scales. *Encyclopedia of Hydrological Sciences* 1–11.
- Hopmans, J.W., Nielsen, D.R., Bristow, K.L., 2002. How useful are small-scale soil hydraulic property measurements for large-scale vadose zone modeling?, in: *Geophysical Monograph Series*. pp. 247–258.
- Hupet, F., Van Dam, J.C., Vanclooster, M., 2004. Impact of Within-Field Variability in Soil Hydraulic Properties on Transpiration Fluxes and Crop Yields: A Numerical Study. *Vadose Zone Journal* 3, 1367–1379.

- Javaux, M., Vanclooster, M., 2006. Scale-dependency of the hydraulic properties of a variably saturated heterogeneous sandy subsoil. *Journal of Hydrology* 327, 376–388.
- Javaux, M., Vanclooster, M., 2004. In Situ Long-Term Chloride Transport through a Layered, Nonsaturated Subsoil. 2. Effect of Layering on Solute Transport Processes. *Vadose Zone Journal* 3, 1331–1339.
- Klute, A., 1986. Water retention : laboratory methods, in: *Methods of Soil Analysis, Part I. Physical and Mineralogical Methods*. 2nd Ed. Edited by Klute, A. 1986. American Society of Agronomy, Madison, Wisconsin, Agronomy Monographs. pp. 635–662.
- Konikow, L.F., 2011. The Secret to Successful Solute-Transport Modeling. *Ground Water* 49, 144–159.
- Labrecque, G., Chesnaux, R., Boucher, M.A., 2020. Water-table fluctuation method for assessing aquifer recharge: application to Canadian aquifers and comparison with other methods. *Hydrogeology Journal* 28, 521–533.
- Lane, K.S., Washburn, D.E., 1946. Capillary tests by capillary meters and by soil filled tubes. *Highway Research Board* 26, 460–473.
- Levitt, D.G., Newell, D.L., Stone, W.J., Wykoff, D.S., 2005. Surface Water-Groundwater Connection at the Los Alamos Canyon Weir Site: Part 1. Monitoring Site Installation and Tracer Tests. *Vadose Zone Journal* 4, 708–717.
- Marshall, T.J., Holmes, J.W., Rose, C.W., 1996. *Soil physics*. Third edition, Soil Physics. Third edition. 3rd ed. Cambridge University Press, Cambridge, U.K.
- Mattei, A., Goblet, P., Barbecot, F., Guillon, S., Coquet, Y., Wang, S., 2020. Can soil hydraulic parameters be estimated from the stable isotope composition of pore water from a single soil profile? *Water (Switzerland)* 12, 1–19.

- Mattern, S., Vanclouster, M., 2010. Estimating travel time of recharge water through a deep vadose zone using a transfer function model. *Environmental Fluid Mechanics* 10, 121–135.
- Mohanty, B.P., Shouse, P.J., Miller, D.A., Van Genuchten, M.T., 2002. Soil property database: Southern Great Plains 1997 Hydrology Experiment. *Water Resources Research* 38, 1–8.
- Potrykus, D., Gumuła-Kawęcka, A., Jaworska-Szulc, B., Pruszkowska-Caceres, M., Szymkiewicz, A., 2018. Assessing groundwater vulnerability to pollution in the Puck region (Denudation moraine upland) using vertical seepage method, in: *E3S Web of Conferences*. pp. 44, 00147.
- Potter, J., 1965. Water content of freshly fallen snow. Rep. CIR-4232, TEC-569, Meteorological Branch, Department of Transport, Toronto (Ontario) Canada.
- Richards, L.A., 1931. Capillary conduction of liquids through porous mediums. *Journal of Applied Physics* 1, 318–333.
- Rimon, Y., Dahan, O., Nativ, R., Geyer, S., 2007. Water percolation through the deep vadose zone and groundwater recharge: Preliminary results based on a new vadose zone monitoring system. *Water Resources Research* 43, 1–12.
- Sauerbrey, I.I., 1932. On the problem and determination of the permeability coefficient. *VNIIG Proceedings* 3–5.
- Schaap, M.G., Leij, F.J., Van Genuchten, M.T., 2001. Rosetta: A computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. *Journal of Hydrology* 251, 163–176.
- Šimůnek, J., Bradford, S.A., 2008. *Vadose Zone Modeling: Introduction and Importance*.

- Vadose Zone Journal 7, 581–586.
- Sprenger, M., Erhardt, M., Riedel, M., Weiler, M., 2016. Historical tracking of nitrate in contrasting vineyards using water isotopes and nitrate depth profiles. *Agriculture, Ecosystems and Environment* 222, 185–192.
- Sprenger, M., Volkmann, T.H.M., Blume, T., Weiler, M., 2015. Estimating flow and transport parameters in the unsaturated zone with pore water stable isotopes. *Hydrology and Earth System Sciences* 19, 2617–2635.
- Stumpp, C., Hendry, M.J., 2012. Spatial and temporal dynamics of water flow and solute transport in a heterogeneous glacial till: The application of high-resolution profiles of $\delta^{18}\text{O}$ and $\delta^2\text{H}$ in pore waters. *Journal of Hydrology* 438–439, 203–214.
- Stumpp, C., Maloszewski, P., Stichler, W., Fank, J., 2009. Environmental isotope ($\delta^{18}\text{O}$) and hydrological data to assess water flow in unsaturated soils planted with different crops: Case study lysimeter station “Wagna” (Austria). *Journal of Hydrology* 369, 198–208.
- Szymkiewicz, A., Gumuła-Kawęcka, A., Potrykus, D., Jaworska-Szulc, B., Pruszkowska-Caceres, M., Gorczewska-Langner, W., 2018. Estimation of conservative contaminant travel time through vadose zone based on transient and steady flow approaches. *Water (Switzerland)* 10, 1417.
- Thomas, E.M., Lin, H., Duffy, C.J., Sullivan, P.L., Holmes, G.H., Brantley, S.L., Jin, L., 2013. Spatiotemporal Patterns of Water Stable Isotope Compositions at the Shale Hills Critical Zone Observatory: Linkages to Subsurface Hydrologic Processes. *Vadose Zone Journal* 12, 1–16.
- Tremblay, P., 2005. Étude hydrogéologique de l’aquifère de Saint-Honoré avec emphase

sur son bilan hydrique [Hydrogeologic analysis of Saint-Honoré aquifer with emphasis on its water budget]. Master's Thesis, Université du Québec à Chicoutimi, Québec, Canada.

Van Genuchten, M.T., 1980. A Closed-form equation for predicting the hydraulic conductivity of unsaturated soils¹. *Soil Science Society of America Journal* 44, 892–898.

Vereecken, H., Schnepf, A., Hopmans, J.W., Javaux, M., Or, D., Roose, T., Vanderborght, J., Young, M.H., Amelung, W., Aitkenhead, M., Allison, S.D., Assouline, S., Baveye, P., Berli, M., Brüggemann, N., Finke, P., Flury, M., Gaiser, T., Govers, G., Ghezzehei, T., Hallett, P., Hendricks Franssen, H.J., Heppell, J., Horn, R., Huisman, J.A., Jacques, D., Jonard, F., Kollet, S., Lafolie, F., Lamorski, K., Leitner, D., McBratney, A., Minasny, B., Montzka, C., Nowak, W., Pachepsky, Y., Padarian, J., Romano, N., Roth, K., Rothfuss, Y., Rowe, E.C., Schwen, A., Šimůnek, J., Tiktak, A., Van Dam, J., van der Zee, S.E.A.T.M., Vogel, H.J., Vrugt, J.A., Wöhling, T., Young, I.M., 2016. Modeling Soil Processes: Review, Key Challenges, and New Perspectives. *Vadose Zone Journal* 15, 1–57.

Vero, S.E., Healy, M.G., Henry, T., Creamer, R.E., Ibrahim, T.G., Richards, K.G., Mellander, P.E., McDonald, N.T., Fenton, O., 2017. A framework for determining unsaturated zone water quality time lags at catchment scale. *Agriculture, Ecosystems and Environment* 263, 234–242.

Vukovic, M., Soro, A., 1992. Determination of hydraulic conductivity of porous media from grain-size composition. *Water Resources Publications*, Littleton, Colorado.

Wentworth, C.K., 1922. A scale of grade and class terms for clastic sediments. *Journal of*

Geology 30, 507–521.

Western, A.W., Grayson, R.B., 1998. The Tarrawarra data set: Soil moisture patterns, soil characteristics, and hydrological flux measurements. *Water Resources Research* 34, 2765–2768.

Zappa, G., Bersezio, R., Felletti, F., Giudici, M., 2006. Modeling heterogeneity of gravel-sand, braided stream, alluvial aquifers at the facies scale. *Journal of Hydrology* 325, 134–153.

FIGURE CAPTIONS:

[Figure 1](#). Vertical VWC profile through the investigated vadose zone.

[Figure 2](#). Grain-passing percentages versus sieve-opening diameter for the sediment samples.

[Figure 3](#). Identified sediment fraction through the investigated vadose zone.

[Figure 4](#). Water table levels as recorded in piezometer PZ-1 over a full year (onward from 9 November 2016). Reproduced from [Labrecque *et al.* \(2020\)](#).

[Figure 5](#). Variation of the adjusted daily cubic water flux used as the upper boundary condition.

[Figure 6](#). Measured and simulated VWC profiles.

[Figure 7](#). Tracking particle depth–distance for (a) 0.36 years, (b) 0.72 years, (c) 0.88 years, and (d) 1 year. The blue vertical lines within the columns indicate the particle pathway.