Table 2. Thermal properties of basement floor material.					
Material	Density	Specific Heat	Thermal		
	(kg/m^3)	Capacity	Conductivity		
		(J/kg-K)	(W/m-K)		
Concrete	2300	880	1.8		
Insulation	34	1450	0.041		



Figure 1.	3-D	view	of g	eometrv	of th	e model.
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Month	Cooling	Heating
(-)	(MWh)	(MWh)
January	19	75
February	18	60
March	23	49
April	27	24
May	29	12
June	38	5
July	50	2
August	48	4
September	38	11
October	30	23
November	22	46
December	20	68

Table 3. Heating and cooling demand of SPEB.

3 MODEL SET-UP

The 3-D model presented in this section is aimed at investigating the thermal performance of a hypothetical geothermal pile foundation system using COMSOL Multiphysics for the SPEB. The energy integrity of the thermal piles is studied by considering the potential impact of energy loss through the below-grade envelop of SPEB. The heat transfer in the model is governed by the ambient air temperature, properties of the insulation layer and concrete material which are

assumed to be constant and also thermal properties of the soil in which phase change occurs due to temperature decrease below the freezing point. It is assumed that all of the 119 vertical piles, which have a 400 mm diameter and support the structural load of the building, are GHEs. The dimensions of the soil domain in which piles are installed are 44 m \times 34 m \times 1 0m (Figure 1).

3.1 Governing Equations of the Thermal Analysis

The transient heat transfer in the insulation layer, concrete slab, piles and pile caps which are modeled as solid domains is governed by the following equation:

$$\rho C_P \frac{\partial T}{\partial t} + \nabla . q_c = Q$$
^[1]

where, ρ (kg/m³) is the density, C_p (J/kg-K) is the material's specific heat capacity, t represents the time (s), T (°C) is the temperature and Q (W/m³) is the heat source. In this numerical modelling, the heat source is the heat extracted/injected from/into the ground with the GHEs. Moreover, q_c is the conductive heat flux which based on Fourier's law can be defined as follow:

$$q_c = -\lambda \nabla T \tag{2}$$

in which λ is the material's thermal conductivity and ∇ represents the gradient operator. As mentioned earlier, heat transfer in the ground in which phase change occurs depends on latent heat of freezing when the temperature decreases below the freezing temperature. As such, considering soil to be saturated and negligible volume change of water during freezing, heat transfer in the soil is governed by the following equation (Zhu and Michalowski 2004):

$$\rho C_{P} \frac{\partial T}{\partial t} - L_{f} \rho_{i} \frac{\partial \theta_{i}}{\partial t} + \nabla q_{c} = Q$$
[3]

where L_f is the heat of fusion per unit mass of water (333 kJ/kg), ρ_i is the density of ice, θ_i is the ice volumetric fraction. The product ρC_p represents the soil's volumetric heat capacity which is calculated by the summation of the volumetric heat capacity of each constituent of the soil (i, e., solid skeleton, ice and water) taking into account their volumetric fraction as described by the following equation:

$$\rho C_P = \rho_w C_w \theta_w + \rho_i C_i \theta_i + \rho_s C_s \theta_s$$
[4]

To determine the thermal conductivity of the freezing soil, the following equation can be used:

$$\lambda = \lambda_w \theta_w + \lambda_i \theta_i + \lambda_s \theta_s$$
^[5]

where in Equation 4 and 5, s, i and w subscripts identify the solid skeleton, ice and water. As the ground temperature decreases below the freezing point (T₀), pore water starts freezing. However, some fraction of water remains liquid even at a temperature below T₀. The volumetric fraction of ice in the pores can be estimated by the following equation (Zhu and Michalowski 2004):

$$\theta_{i} = \theta_{w0} - \left[\theta_{wr} + \left(\theta_{w0} - \theta_{wr}\right)e^{a(T-T_{0})}\right]$$
[6]

where θ_{wr} is the residual unfrozen water content faction [-] at a given temperature below freezing point equal to 0.05 [-], θ_{w0} is the initial unfrozen water content fraction [-], and *a* (1/K) is a constant for controlling the curvature equal to 0.16 (Zhu and Michalowski 2004).

3.2 Boundary Conditions

To evaluate the impacts of seasonal temperature variation on temperature distribution of the ground, a convective heat flux has been defined for the top boundary of the model surrounding the building's plan using the following equation:

$$q_{conv}(t) = h_{conv}\left(T_{air}(t) - T_s(t)\right)$$
^[7]

where *h* is the convective heat transfer coefficient which is equal to $6 \text{ W/m}^2\text{-K}$ in this study (Bobko et al. 2018). T_{indoor} denotes indoor temperature of the building's basement which is assumed to be kept constant by the HVAC system and equal to 20 °C. In urban areas, subsurface temperature profile is higher than an open field (Fergusen and Woodbury 2004) due to the buildings' energy loss through their below-grade enclosure. As such, the initial temperature distribution of the soil domain in this study is speculated to be time and depth dependent. To determine the initial temperature profile of the current 3D model, a separate thermal analysis has been done over a 30-year span of time (i. e., 1988-2018) in which the ground surface at the construction site is in direct contact with the ambient air and the impact of the adjacent buildings' heat leakage on the ground temperature has been evaluated.



Figure 2. View of the surface of the 3D model developed for obtaining the ground's initial temperature profile.

The surface of the 3D model developed in COMSOL Multiphysics (Figure 2) is made of several regions: region 4 is the construction site of the SPEB which is surrounded by the previously constructed areas (i.e.: regions 1, 2 and 3). To simulate the energy loss through the surrounding structures' basement, a convective heat flux based on Equation 7 is defined for the regions 1 to 3. The boundary condition assigned to the non-constructed regions (i.e.: regions 4, 5 and 6) is a convective heat flux with the ambient air according to Equation 6. After implementing the model as described, the results from the 30-year thermal analysis have been then assigned as the initial temperature distribution of the soil domain (Figure 1).

The ground temperature distributions in two cross-sections of the soil domain before the SPEB construction are shown in Figure 3. Based on the results of numerical modelling, the ground temperature in the cross-section 7 m away from to the Western boundary of the model

(Figure 3a) is up to 5 °C higher than ground temperature at the center of the region 4 of the soil domain (Figure 3b). Therefore, ground temperature of the regions underneath the constructed areas (i.e.: eastern and south western boundaries) is higher than ground temperature of the regions underneath open areas.



Figure 3. Ground temperature distribution before the SPEB construction from 4 to 14 m below ground surface along vertical cut planes at (a) 7 m away from the east boundary (i.e. Section A) and (b) the center of the region 4 of the soil domain (i.e. Section B).



Figure 4. Ground temperature distribution 5 years after construction of the SPEB from 4 to 14 m below ground surface along vertical cut planes at (a) 7 m away from the west boundary (b) the center of the region 4 of the soil domain.

4 RESULTS

The design of energy efficient building has been gaining attention to decrease the energy loss through buildings envelope and improve their energy efficiency. However, most efforts for decreasing the energy loss are focused on the above-grade envelope while significant energy losses can occur through the below-grade enclosure of a building. As such, to assess the effect of energy loss through the floor slab after construction of the building on the ground temperature, thermal performance of the basement is investigated for five years. As shown in Figure 4 for the same cross-sections as in Figure 3, despite insulating the basement's floor slab, after five years, ground temperature especially close to the surface increased noticeably comparing to the initial

ground temperature.

As mentioned earlier, in cold regions such as Canada, the annual heat extraction shall be higher than heat injection from/to the ground which contributes to subgrade thermal imbalance. As a result, a thermal pile system is doom to fail after few years due to the cooling of the ground from year to year and no more heat to extract from the ground. However, in the case of the SPEB, the heating and cooling loads are different (Table 3) and the net year-round heat production of the building is positive. Based on the analysis of the geothermal energy pile foundation system after a five-year operation (Figure 4), there is a thermal imbalance in the ground and the ground is warming over time. The thermal load of each pile is then a heat source. The assumption taken for estimating the magnitude of heat source is that the piles are functioning within a GSHP system which has a constant coefficient of performance (COP) of 3. A constant COP for the system is a conservative assumption in which the possibility for the highest ground temperature to decrease can be assessed. Knowing the energy demand of the building and COP of the system, the magnitude of heat source can be calculated using Equation 8.

$$Q_c = Q_H \left(1 - \frac{1}{COP} \right)$$
[8]

in which Q_c is the extracted heat from the ground using the geothermal foundation and Q_H is the supplied heat to SPEB by the heat pump that, in the present work, is equal to the heat demand of the building during winters and cold demand during summers. In Equation 8, Q_c and Q_H with a negative sign denotes the cooling load of the building.

As shown in Figure 5, over a five-year period of operation of the SPEB, the ground temperature at a depth of 8 m below the basement level decreases by almost 3.5°C. However, the seasonal variation of ground temperature close to the basement level follows a steady trend over the five-year period of operation of the SPEB. This is due to the additional heat which is lost into the ground from the SPEB's below-grade enclosure. Such heat loss mostly impacts the ground temperature close to the basement level.



Figure 5. Ground temperature as a function of time at depths of 2, 5, and 8 m below the basement level of the SPEB over a five-year period of operation.

As shown in Figure 6a, due to excessive heat extraction, soil may freeze at the surface of the pile which may lead to frost heaving during cold season. Once the system starts injecting heat to the ground, thawing occurs and consequently thaw settlement may occur. Therefore, thermal imbalance not only impacts the energy integrity of GSHP system, but it would affect the structural integrity of geothermal energy pile foundation system as well. The basement floor's

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heat loss favorably impacts thermal imbalance of the ground although in a building such as SPEB with high annual energy demand underground thermal imbalance occurs. As such, mitigation methods need to be implemented to meet the ground thermal balance.



Figure 6. Temperature distribution surrounding the piles located underneath the basement at (a) the end of the cold season of the fifth year and (b) the end of the hot season of the fifth year of the operation period of the SPEB.

5 CONCLUSION

In present work, the feasibility of applying a geothermal foundation system is assessed for supplying the monthly energy demand of the Stanley Pauley Engineering building (SPEB) for space heating and cooling. This is done through a five-year thermal analysis of the ground underneath the SPEB considering the impacts of the energy loss through the basement envelope. According to the results, the following conclusions can be drawn:

- Heat loss through the basement enclosure significantly increases the ground temperature. Such heat loss can be re-harvested by the geothermal pile foundation system.
- In the case of fully supplying the building's energy demand using geothermal energy foundation, thermal imbalance occurs in the ground. Such thermal imbalance mostly impact soil at deeper level since basement's heat loss compensate for excessive heat extraction at shallower levels. However, to be able to support the building's energy demand only by geothermal energy, it is believed that auxiliary heat source units need to be considered.

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Chloride Diffusion in Cement Materials at Different Leaching States: An Experimental and Numerical Study

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ABSTRACT

Due to common heavy snowfall in winter, concrete structures in cold countries are regularly in contact with water. Hence, concrete undergoes abnormal leaching of ionic species present inside the liquid pores of the material. The leaching slowly degrades the structures and may have an influence on the diffusive properties of the chloride ions, coming from the de-icing salts and responsible for the corrosion of the steel reinforcements present in the reinforced concrete. In this work, an experimental and numerical study is propounded to better understand the influence of the leaching state of cementitious material on the diffusive behaviour of chloride ions. Natural and accelerated diffusion tests were performed on samples of hydrated cement paste and concrete samples with lower chloride concentrations (50 mol/m³). The materials were conserved at different leaching state with care not to degrade the microstructure: safe (S), partially leached (PL), and leached (L). The simulation of those various tests was carried out on the reactive transport software PhreeqC to quantify the chloride diffusion. This numerical model allows distinguishing the influence of the geometry of the material (porosity, tortuosity, constrictivity...) to the chemical reactions occurring between chloride ions and the cementitious phases. It then appeared that chloride ions do not diffuse in the same way depending on the leaching state of the cementitious material. Same observations are made on hydrated cement paste and concrete samples. In a safe material, the chloride ions diffuse slowly than in a leached material. It seems not to be due to the material geometry nor chemical reactions. The numerical model developed confirms this hypothesis as it allows to distinguish and quantify their both influence on the chloride diffusion. This study, therefore, highlights the importance of considering the leaching effects in the prediction model for concrete structure durability in cold countries.

KEY WORDS: Diffusion, chloride, leaching, cement materials, experimental, numeric.

1 INTRODUCTION

For the life structure prediction, that is essential to be able to characterize the cementitious material behaviour face to the diffusion of aggressive substances such as chloride ions. Studies on the diffusion of chloride, from marine or de-icing salt, in cementitious materials, are largely available in the literature (Ait-Mokhtar et al., 2004; Andrade et al., 1994; Castellote et al., 2001; Delagrave et al., 1996; Loche et al., 2005; Nilsson et al., 1996; Ollivier et al., 2002; Tang, 1996; Truc, 2000). For more convenience, all these studies are mainly on a safe concrete prepared for the laboratory test and the numerical model does not consider the degradation of the material. However, the concrete structures in their environment are in contact with water, leading to a

progressive decalcification and degradation of the material microstructure. It is, therefore, necessary to study the diffusion of ionic species on a safe material and at different leaching states to observe the impact of the material leaching state on the diffusion of aggressive substances, such as chloride.

An electro-diffusion test procedure was previously optimized (Sanchez, Ait-Mokhtar, et al., 2018) to reliable observe the chloride diffusion regarding the microstructure and chemical properties. In order to simulate the tests, a numerical model has been created on PhreeqC (Sanchez, Millet, et al., 2018), it manages multi-species diffusion in a reactive environment. The calibration was carried out on hydrated cement pastes with different Water/Cement (W/C) ratio.



Figure 1. European denomination of the different leaching states and identification of the samples used in this work. Stage I: Healthy. Stage II: Leached. Stage III and IV: Microstructure degraded.

The aim of this research is hence to observe the chloride diffusion in cement materials at different leaching state by performing electro-diffusion tests and quantifying the diffusion with a numerical model in PhreeqC. The materials studied have the same microstructure as pH pore solution was controlled to be always upper than 12.5, the only difference between the leaching state studied is the composition of the pore solution of the hydrated cement paste. On the European designation (Figure 1), the following three states are studied: Safe at pH 13.4 (Stage I), Partially Leached at pH 12.9 (Stage I-II) and Leached at pH 12.5 (Stage II).

2 TEST AND METHODS

2.1 Materials and methods

Mix were prepared with Portland cement CEM V (CEM V/A – S-V – 42.5 N CE PM-ES-CP1 NF 'PMF3'). Experimental tests were carried out on hydrated cement pastes with a 0.4 Water/Cement (W/C) ratio and concrete with a 0.37 W/C ratio (Table 1).

The first centimetres of each specimen from the surface was removed to avoid any edge effects and possible milt. Then, specimens were cored and sawed in samples of 65 mm diameter and 10 mm thick. Samples were conserved at a regular temperature (20 $^{\circ}$ C) and at different leaching state, subsequently noted for hydrated cement paste samples:

• CPV-S (Safe Cement Paste V) and CV-S (Safe Concrete V) are stored in a curing solution highly concentrated in alkalis in order not to modify its porous solution;

- CPV-PL (Partially Leached Cement Paste V), after one year of curing, are stored in ultrapure water to reduce the alkaline content of the pore solution for one year;
- CPV-L (Leached Cement Paste V), after one year of curing, are stored in a lime solution ([CaO]= 15.81 mol/m³) for one year. A constant pH of 12.5 is monitored to replace the alkaline porous solution with a concentrated calcium solution without degrading the material. Curing spent at least one year to ensure the complete material saturation. The saturation of the samples was verified by immersion under vacuum in a desiccator for 24 hours.

Tuble It composition of the child v concrete samples (cv)				
Concrete CV	Content (kg/m ³)			
Cement	470			
Water	173			
Filler	78			
Sand	912			
Gravel (4/6mm)	312			
Gravel (6/10mm)	312			
Plasticizer	4.7			

Table 1. Com	position o	of the	CEM V	concrete s	samples ((CV))
			-			· - · /	

Table 2 summarises the water porosities and the ionic chemical compositions of the pore solutions, measured by suspensions, after 2 years of ageing. Concentrations are measured by ionic chromatography Metrohm 930 Compact IC Flex with around 10% accuracy (depending on the ionic species studied and the dilution used for analyses). The normalized pore distribution after 2 years of ageing (Figure 2) highlights the same microstructures for safe and leached hydrated cement paste in accordance with the water porosity measures. Characterization tests hence demonstrate only different pore solution composition between the different material but same geometrical parameters. Compared to a most common hydrated cement paste CEM I W/C 0.42 (CPI-042) (Sanchez, Ait-Mokhtar, et al., 2018; Sanchez, Millet, et al., 2018), the main presence of nanoporosity could greatly influence the ionic diffusion because of capillarity effects. Mercury porosity also demonstrates that the different hydrated cement pastes have similar microstructures then only porosities between safe and leached samples seems to slightly vary.

2.2 Diffusion tests

Electro-diffusion test: The electro-diffusion tests follow the modified procedure (Sanchez, Ait-Mokhtar, et al., 2018). A saturated sample taken from the cure was resin-coated to let the diffusion be one-dimensional. It was placed between two cells: the upstream cell contains 50 mol/m³ of chloride ions (NaCl) in a basic solution composed by potassium hydroxide KOH and sodium hydroxide NaOH with concentrations given by the pore solution study. The downstream cell contains only KOH and NaOH. During the test, the chloride concentration gradient between the two cells influences its transport slowly through the material. To accelerate the process, a constant electrical field was applied to the sample and punctually, two reference electrodes placed at the material bounds allows to verify the potential constancy. The electrical field was fixed to a value corresponding to a weak initial current value around 20–30 mA. Current density passing through the sample was punctually measured along the test with the power supply Hameg HMP4040. The chloride concentration downstream was measured by ionic