ASSESSING ROCK AQUIFER VULNERABILITY USING DOWNWARD ADVECTIVE TIMES FROM A 3D MODEL OF SURFICIAL GEOLOGY

Martin Ross, INRS Eau, Terre et Environnement, Québec, Qc., Canada
Richard Martel, INRS Eau, Terre et Environnement, Québec, Qc., Canada
Michel Parent, Geological Survey of Canada, Québec Office, Québec, Qc., Canada
René Lefebvre, INRS Eau, Terre et Environnement, Québec, Qc., Canada
Martine M. Savard, Geological Survey of Canada, Québec Office, Québec, Qc., Canada

ABSTRACT
An aquifer vulnerability assessment method combining a 3D geologic modeling approach and the notion of Downward Advective Time (DAT) is tested over a 1400 km^2 area in the St. Lawrence Lowlands in southwestern Quebec. To assess the vulnerability of the regional rock aquifer, hydrogeologic parameters such as infiltration rate and porosity of each unit overlying the aquifer were first sampled randomly (200 samples) within their estimated range by applying a script command to a gOcad 3D stratigraphic grid. At the end of each run, the DAT from the surface through this layered system was approximated on 74% of the model area. Then, results were grouped into DAT classes which provide a relative vulnerability index. The mean DAT map is highly consistent with available information. Furthermore, the variation in the high vulnerability zone coverage is small between the different outcomes suggesting that the stratigraphic architecture has a greater impact on the vulnerability assessment at regional scale than the input parameters variability and that the chosen classes are appropriate for the most critical areas.

RÉSUMÉ
Une méthode d'évaluation de la vulnérabilité des aquifères, basée sur la notion de temps advectif vertical (TAV) et l'utilisation d'un modèle géologique 3D, est testée sur une superficie de 1400 km^2 dans les basses terres du Saint-Laurent au sud-ouest du Québec. Pour évaluer la vulnérabilité de l'aquifère rocheux régional, des paramètres hydrogéologiques tels que la vitesse d'infiltration et la porosité de chaque unité ont d'abord été échantillonnés aléatoirement (200 échantillons) à l'intérieur d'une plage réaliste de valeurs, à l'aide d'une série de commandes exécutées dans gOcad sur une grille stratigraphique 3D. À chaque fois, le TAV a été estimé sur 74% de la région. À la fin, les résultats ont été regroupés en classes de TAV afin de définir un indice de la vulnérabilité relative. La carte faite à partir des TAV moyens montre un degré de cohérence élevé avec les informations disponibles. De plus, la superficie des zones de vulnérabilité élevée varie peu entre les différents scénarios suggérant que l'architecture stratigraphique a un plus grand impact sur l'évaluation de la vulnérabilité à l'échelle régionale que la variabilité des paramètres et que les classes sont appropriées pour les zones les plus critiques.

1. INTRODUCTION

Accessibility to consistent subsurface stratigraphic information is crucial to map the vulnerability of aquifers overlain by several discontinuous units but it is often the missing link at regional scale. In the last decade, however, geoscientific databases as well as different geomodeling tools (e.g., gOcad, EarthVision) and approaches have been developed and/or improved to better allow the construction of detailed 3D geologic models (e.g., Soller et al. 1999; Ross et al. in press, a) in a way that standard GIS or CAD tools simply cannot do (e.g., Mallet 2002). The increasing accessibility to this technology has opened a new perspective in regional hydrogeology and many Geological surveys have started 3D mapping programs to provide the most detailed and consistent stratigraphic information in rapid-growth areas where the population mainly relies on groundwater for its water supply (e.g., Berg 2000; Berg et al. 2004; http://www.isgs.uiuc.edu/...). Few 3D models are available in Canada but it is expected to improve in the near future. These 3D geologic models have the potential to provide more consistent data for unit distribution and thickness than the GIS-based multi-layered models and they can also integrate information about soil properties and hydrogeologic parameters at various scales of resolution. Therefore, once it is available, a 3D geologic model can be very useful to map aquifer vulnerability to contamination.

Among the most interesting methods to use with a detailed 3D geologic model are those that relate the vulnerability directly to a parameter that expresses a physical property. In the AVI method (Van Stempvoort et al. 1993), for example, the aquifer vulnerability is considered to be inversely related to the bulk hydraulic resistance of the layered system above the aquifer. A slightly different approach was considered and successfully tested recently in southwestern Québec on a 3D geologic model (Ross et al. 2003; in press, b). In contrast to the AVI method, which could also be easily applied on a 3D geologic model, this method relates the vulnerability to Downward Advective Times (DAT) estimated with Darcy's law, rather than with the hydraulic resistance factor.

The main objective of this paper is to present additional testing to an approach at mapping aquifer vulnerability at regional scale from groundwater DAT estimated using a

3D geologic model that integrates a few key input parameters (Ross et al. 2003; in press, b). The purpose of this additional testing phase is to verify the impact of uncertainty and/or heterogeneity associated to some of the input parameters used in the vulnerability assessment. In this case study, the groundwater DAT are estimated from the surface through discontinuous and unconsolidated Quaternary units to an underlying fractured rock aquifer.

2. STUDY AREA

The study area extends over about 1500 km^2 between the Laurentian Highlands, the Ottawa River and other St. Lawrence River tributaries (Figure 1). The bedrock is essentially made of Paleozoic sedimentary rocks of the St. Lawrence Lowlands Platform, which locally consists of a succession of sandstones and carbonates ranging from Cambrian to Middle Ordovician (Globensky 1987). These rocks are underlain by a Precambrian basement which outcrops in the Laurentian Highlands as well as in two hills (St. André and Oka) which also contain Cretaceous alcaline intrusions. Bedrock is overlain by a discontinuous cover of Quaternary sediments reaching up to 150 m in thickness. The Quaternary sequence mainly comprises Late Wisconsinan subglacial (20-12 ka), proglacial (12-10 ka) and Holocene (<10 ka) postglacial sediments. Till and Champlain Sea silt and clay are the most widespread sediments (Bolduc and Ross 2001a, 2001b; Ross et al. 2001). The Quaternary succession largely controls the confining conditions of the regional aquifer as well as its recharge, which occurs on topographic highs where bedrock either crops out or is covered by a discontinuous till sheet of variable thickness. Figure 2 shows the general hydrostratigraphic framework of the study area.

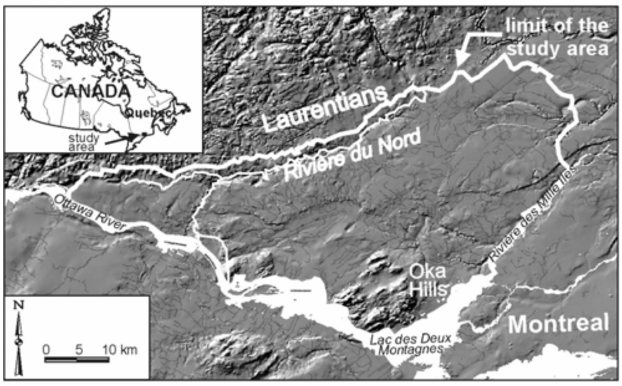

Figure 1: Location of study area with digital elevation model as background.

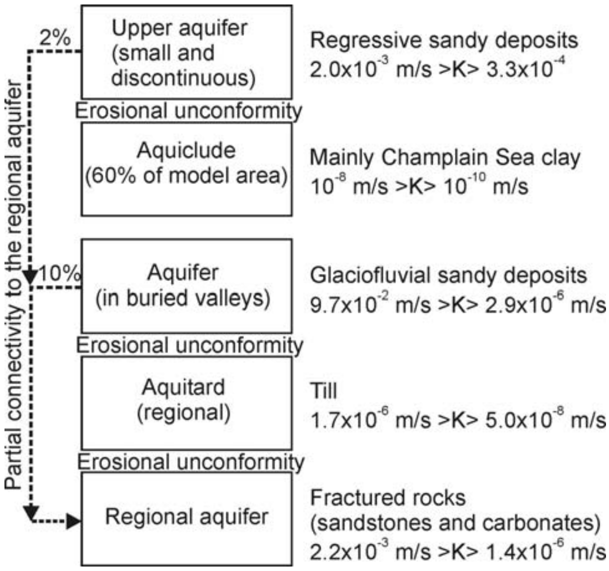

Figure 2: General hydrostratigraphic framework (K: hydraulic conductivity). A total of 12% of the model area shows direct vertical hydraulic connection between discontinuous granular aquifers and the regional rock aquifer (cf., Ross et al. in press, b).

3. METHODS

3.1 3D geologic modeling

Many approaches to 3D geologic modeling exist and theoretical background as well as currently-used methods are described in a few references (e.g., Turner 1992; Mallet, 2002). The model used in this work was constructed using the geomodeling software gOcad 2.0.4 and subsequent versions (Earth Decision Sciences, 2001). The model covers an area of about 1400 km^2 and is made of interlocked discontinuous triangulated surfaces representing the top of each of the main Quaternary units of the basin as well as bedrock topography. It is a grid-independent model which may be internally meshed in different ways. For a more complete description of the procedure used to construct the model, the reader is referred to Ross et al. (in press, a).

3.2 The aquifer vulnerability method

A method was proposed by Ross et al. (2003; in press, b) that makes use of a 3D geologic model and allows for a relative regional estimate of aquifer vulnerability to downward transport of dissolved and persistent contaminants based on groundwater DAT. It usually requires a full 3D numerical flow model to estimate groundwater time-of-travel (TOT) but these sophisticated numerical models would be difficult to implement as a groundwater vulnerability evaluation tool on a regional scale and it may not necessarily provide more reliable outputs to specifically estimate vulnerability. Moreover, in many instances the assessment complexity can be greatly reduced by treating the TOT estimation as a one-dimensional advective flow problem with potential contaminant moving vertically downward. Here, the aim is to estimate groundwater DAT from the surface through a regional geologic model to the underlying regional aquifer. It is apparent that such an approach is a simplification of the real complexity of the system but it is assumed that reasonable estimates are possible as long as the interpretation of results is made within the limitations of the adopted simplifying assumptions. The main assumptions are summarized below:

1) The relative vulnerability of an aquifer can be obtained by estimating DAT using geologic and hydrogeologic information;
2) Factors that may change over time such as land use or seasonal effects are not considered;
3) Contaminant behavior is the same as water;
4) Contaminants are released at the land surface;
5) Groundwater flow is vertical along the entire length considered for DAT estimation.

The main advantages of this approach are that few input parameters are needed and the method can be applied on a detailed 3D geologic model without significant transformation or adaptation.

The one-dimensional advective, nonreactive, solute time-of-travel or, more simply, the DAT through an unsaturated layered system can be approximated by the following equation:

$$\mathrm{DAT} = \frac{1}{q}\sum_{i=1}^{n} m_i \theta_i \qquad [1]$$

where q (m/s) is the groundwater recharge rate, m_i (m) and θ_i (mL cm^{-3}) are the thickness and volumetric water contents, respectively, of layers at every location where the calculation is applied (Haith and Laden 1989). The sum of m_i is limited by the travel distance D (m) which is usually from the land surface to the top of the evaluated aquifer. Also, when assuming saturation through D, θ is replaced in Eq. 1 by the porosity n (cm^3 cm^{-3}). This applies when the targeted aquifer is largely overlain by saturated less permeable units.

3.2.1 Travel distance and parameter estimation

In the study area, till and marine clay are by far the most abundant Quaternary sediments and they are generally less permeable than the underlying fractured rocks. The rocks act as the regional aquifer, thus, forcing near vertical flow within the saturated overlying less permeable units. Such a process was demonstrated in the classical work of Freeze and Whiterspoon (1967). Therefore, considering vertical flow through the saturated zone above the rock aquifer is a reasonable assumption and DAT were thus estimated for a travel distance starting at the land surface through the Quaternary sequence to the regional fractured rock aquifer. The entire layered system was considered saturated. Also, it was found that the specific discharge exceeds the infiltration rate in all units, except for the regional confining layer (marine clay). Therefore, q was considered equal to the infiltration rate of the uppermost unit except where the marine clay is present and is more than 1 m thick. In this case, q was determined according to the following equation that is equivalent to Darcy's law:

$$q = K_{cl}\frac{\partial h}{TH\_cl}\text{; where } \partial h = h_{surf} - h_r \qquad [2]$$

where TH_cl (m) is the thickness of the confining layer (marine clay), K_{cl} is the hydraulic conductivity of the confining layer, whereas ∂h corresponds to the hydraulic head loss between the surface and the bedrock aquifer. h_{surf} (m) is the topographic elevation minus 2 m, which is the approximated hydraulic head in the surface aquifer or aquiclude, and h_r (m) is the hydraulic head of the rock aquifer (Paradis 2002).

In the initial development phase (Ross et al. 2003, in press, b), a single value was chosen for each input parameter and Eq. 1 was applied once to produce a deterministic estimate. In this paper, the groundwater recharge rates and the porosities of each unit as well as the hydraulic conductivity of the confining layer were chosen randomly within their estimated range (Table 1) and Eq. 1 was applied several times to produce multiple outcomes.

Table 1. Estimated range values for the input parameters.

Unit name	Infiltration rate (mm/y)[1] min, mode, max	Porosity (cm^3 cm^{-3})[2]
Regressive sand (upper aquifer)	175, 240, 300	0.25-0.45
Marine clay [3] (aquiclude)	50, 95, 150	0.35-0.55
Glaciofluvial sediments (aquifer)	200, 300, 400	0.25-0.35
Till (aquitard)	100, 170, 200	0.15-0.30
Undifferentiated sediments (aquifer)	N/A	0.25-0.50
Fractured rock (regional aquifer)	100, 190, 300	0.005-0.05
Hydraulic conductivity (marine clay)	10^{-10}, 10^{-9}, 10^{-8} m/s	

[1]adapted from Hamel (2002)
[2]adapted from literature (e.g., Freeze and Cherry 1979)
[3]applied where clay exposed at surface is ≤ 1 m thick

3.2.2 Geologic model discretization and data processing

The 3D geologic model is primarily defined by a series of interlocking surfaces representing the boundaries of geological objects. With the geomodeling package gOcad, such a framework can be further discretized in different ways to adapt to the specific needs of various applications. In this work, the initial geologic framework was used to generate a curvilinear regular 3D grid that maintains the geometric integrity defined by the interlocked surfaces. Node spacing used in the x and y directions is 200 m and their x and y locations are identical to the grid which provided h_r values used in Eq. 3. After "deactivating" the grid cells located over areas of upward flow and in incomplete 3D model parts, a script command was applied to automatically populate the remaining "active" cells with the input parameters. This process was achieved using a random function that was constrained to choose a value within a distribution defined by three parameters (min, mode, max) for each unit (Table 1) while considering the rules previously described as well as Eq. 2. Two hundred samples were obtained for each parameters and Eq. 1 was applied to generate 200 DAT estimates on the rock aquifer meshed layer (24 890 active cells). Each outcome was stored in an external file for post-processing. The statistics, such as the mean, were calculated and the results were imported back into the grid. Figure 3 illustrates the general procedure.

The "active" cells were grouped in different DAT classes and interpreted in terms of a relative vulnerability index (Table 2). The proposed index allows for a practical, although subjective, ranking of the classes, which is adapted from the one proposed by the Geologic Sensitivity Workgroup (1991). Finally, a few vulnerability maps were generated to show different scenarios.

Table 2. Groundwater DAT classes and the aquifer vulnerability index (from Ross et al. 2003; in press, b).

Groundwater downward DAT (years)	Relative vulnerability index
Less than 0.5 y (class 1)	Very high
0.5 to 5 y (class 2)	High
5 to 20 y (class 3)	Moderate to high
20 to 50 y (class 4)	Moderate
50 to 100 y (class 5)	Low
over 100 y (class 6)	Very low
Areas of upward flow	Very low

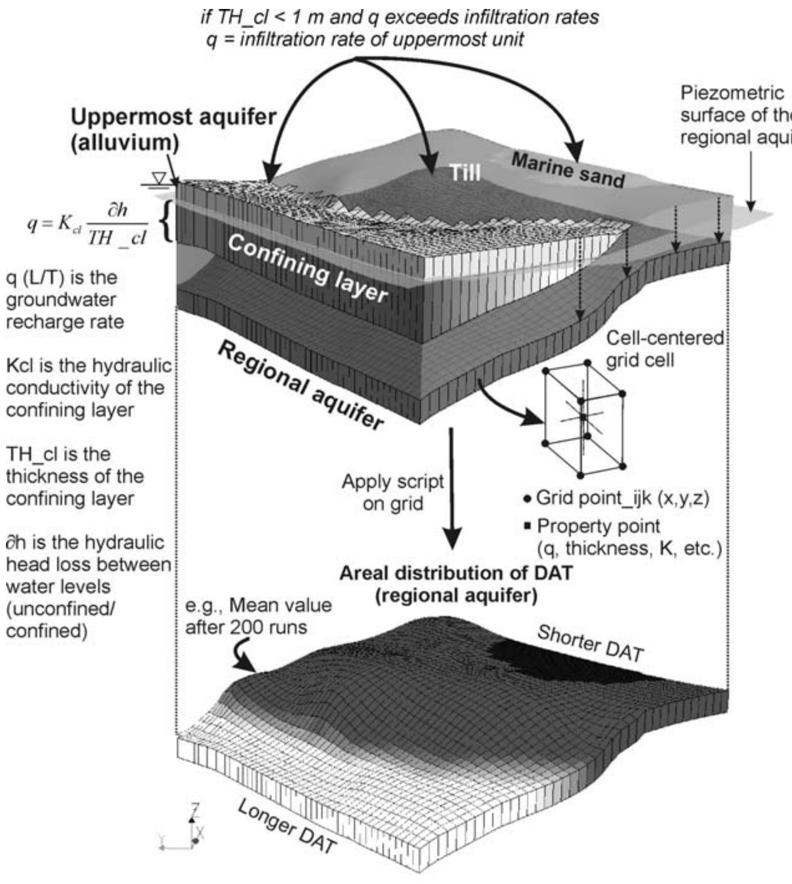

Figure 3. A 3D grid is generated from the geologic model and a script command is applied to integrate input parameters and to estimate DAT from the surface to the underlying regional aquifer (adapted from Ross et al. in press, b).

4. RESULTS AND DISCUSSION

Mean DAT were grouped according to the classes (Table 2) and a vulnerability map was produced to show the results (Figure 4). The map is highly consistent with available information, such as with the distribution of groundwater recharge areas, groundwater type zones of Cloutier and Bourque (2002) as well as areas where contamination from road salt application is known. However, by plotting the mean DAT with the average deviation from the mean, it becomes obvious that there is some overlap between the classes (Figure 5). This indicates that the variability, and/or uncertainty, in the input parameters is large enough to have an impact on the vulnerability map. However, this overlap is quite negligible for classes representing short DAT (Figure 5a) and is significant only for class 5 and class 6 (e.g., Figure 5b). From a land management perspective, the overlap may thus not be highly problematic because the conservation effort will more likely be focused in the more vulnerable areas that are better constrained.

To further analyse the impact of the overlap in the vulnerability assessment, two maps representing extreme cases were generated to see where the most significant changes occur in the study area. Figure 6 shows a map based on the mean DAT minus the average deviation (pessimistic scenario), whereas Figure 7 shows a map based on the mean DAT plus the average deviation (optimistic scenario). In the pessimistic scenario, large zones which are classified as very low vulnerability (class 6) on the mean DAT map have been reclassified as low or moderate vulnerability zones (class 5 or 4). However, only about 3% of the "active" cells have experienced a shift from class 3 to class 2.

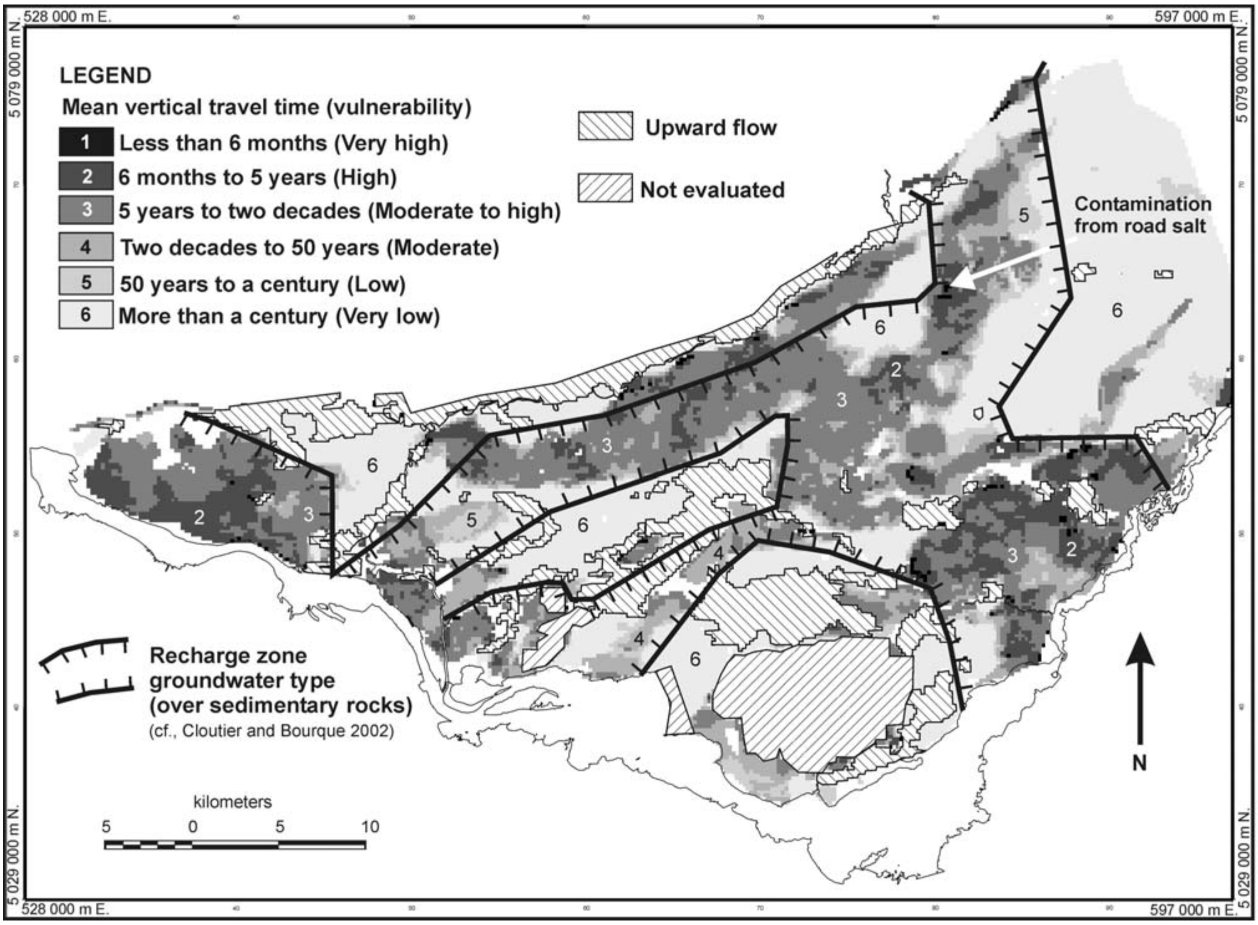

Figure 4. Vulnerability map of the regional rock aquifer in the study area based on the mean DAT. The results are consistent with the available information such as with the distribution of groundwater recharge areas, groundwater type zones and with areas where contamination from road salt application is known.

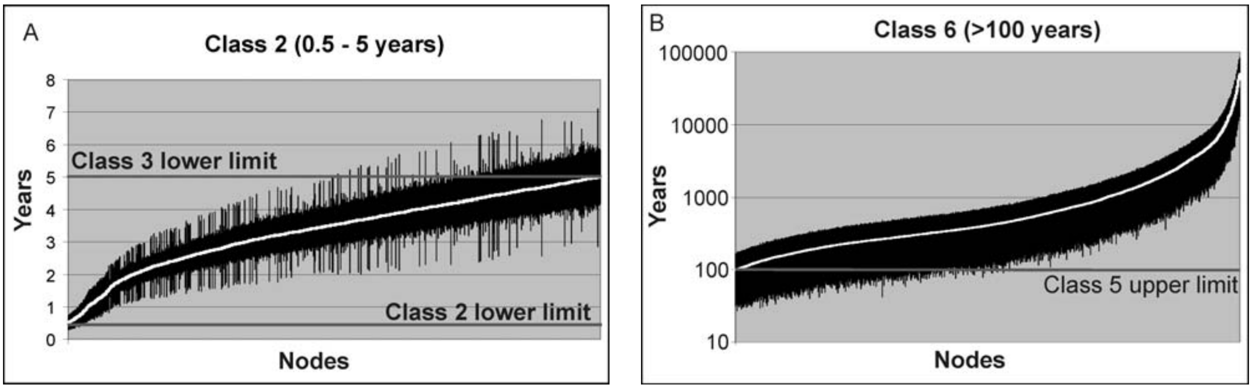

Figure 5. A) Mean DAT (white curve) in ascending order from 0.5 to 5 years (class 2) with associated average deviation showing minor overlap with class 3; B) Mean DAT (white curve) in ascending order starting at 100 years (class 6) with associated average deviation showing more significant overlap with class 5.

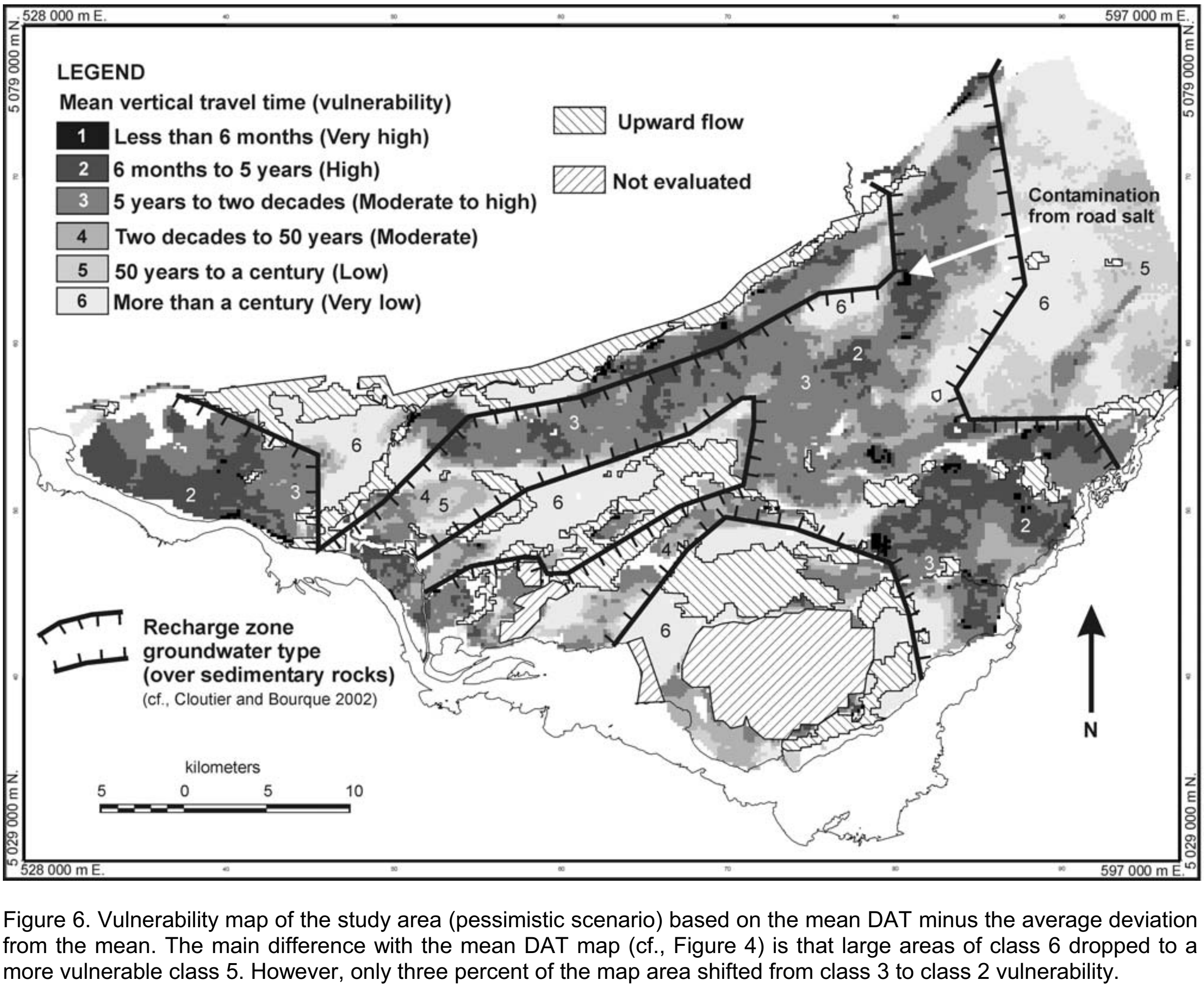

Figure 6. Vulnerability map of the study area (pessimistic scenario) based on the mean DAT minus the average deviation from the mean. The main difference with the mean DAT map (cf., Figure 4) is that large areas of class 6 dropped to a more vulnerable class 5. However, only three percent of the map area shifted from class 3 to class 2 vulnerability.

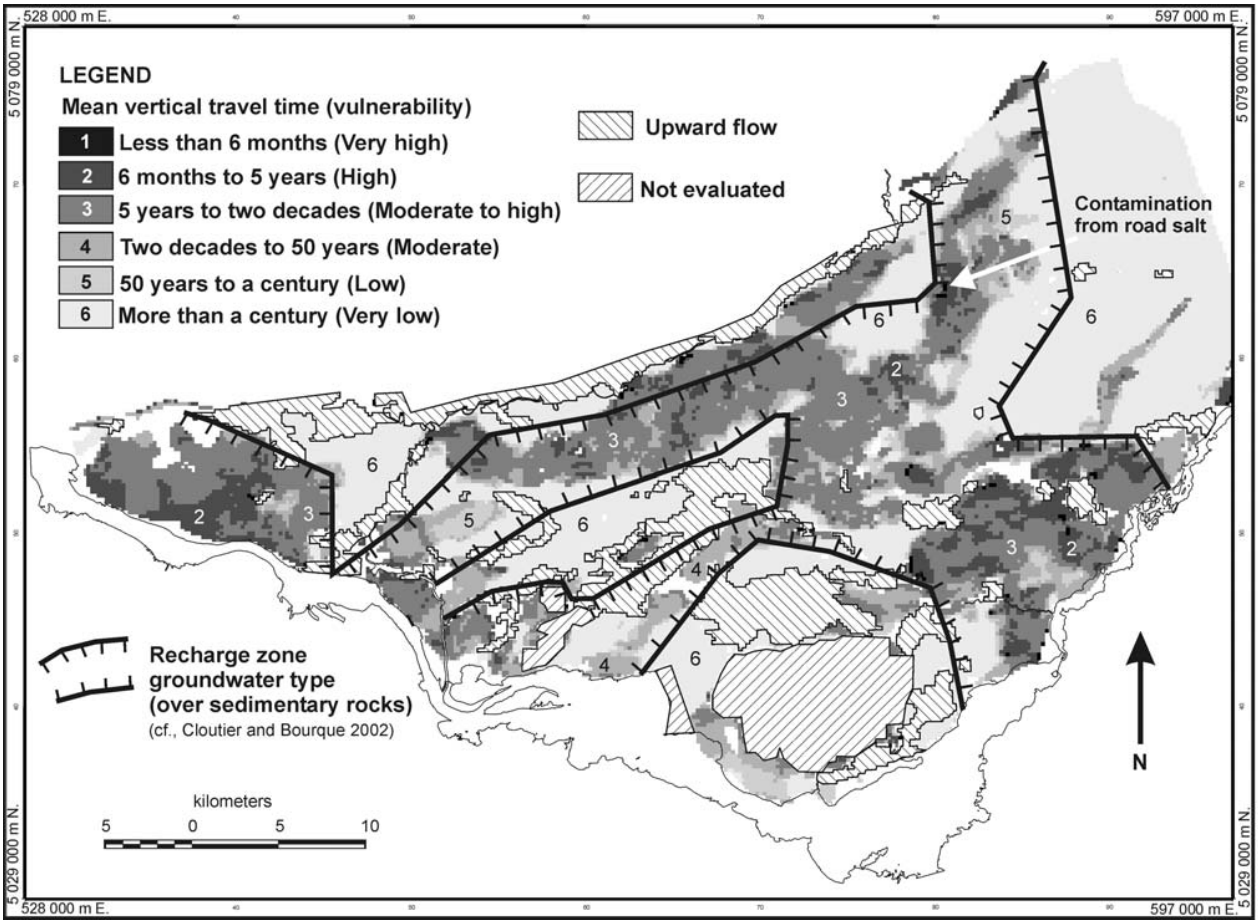

Figure 7. Vulnerability map of the study area (optimistic scenario) based on the mean DAT plus the average deviation from the mean. By comparing with the mean DAT map (cf., Figure 4), only 3% of the map area shifted from class 2 to class 3 vulnerability.

In the optimistic scenario, only about 3% of the "active" cells have shifted from class 2 to class 3. Therefore, the high vulnerability zones are well constrained over the study area. In fact, by considering the 200 outcomes, 35% of the "active" cells have a probability of 0.9 or greater of being within the high vulnerability zone (class 1 to 3), whereas this percentage only increases up to 46% when considering a probability equal or greater to 0.1. This small difference (11%) suggests that the high vulnerability zones are more constrained in the study area by the regional 3D stratigraphic architecture rather than by input parameters variability.

Upcoming developments will focus on improving the script command to streamline the external data storage and post-processing procedures to facilitate more script runs (~ 1000) and be more statistically confident.

5. CONCLUSION

Regional aquifer vulnerability assessments constitute a key part of preventive actions against aquifer contamination. Yet, very few assessment methods are based on a parameter that has a real physical meaning and the subsurface stratigraphic information is often the missing link in this type of assessment. However, 3-D geomodeling is expected to become a standard in the near future. This will improve interactions among the different specialists and end-users and will eventually lead to better integration of geological information in the management of groundwater resources and associated decision-making processes. It is with such a perspective that a new method is being developed to evaluate aquifer vulnerability to downward contaminant transport using a 3D geologic model and a few input parameters. It can be applied in different hydrogeologic settings but it is best suited for cases where the regional aquifer is overlain by several discontinuous layers.

ACKNOWLEDGMENTS

The work was carried out in collaboration with the Geological Survey of Canada (GSC) and it was supported by Natural Resources Canada, Economic Development

Canada, Conseil Régional de Développement-Laurentides, Ministère de l'Environnement du Québec, Ministère des Transport, and the Regional County Municipalities of Argenteuil, Deux-Montagnes, Mirabel and Thérèse-de-Blainville. Financial support to the first author was provided through scholarships from the Fonds Québécois de la Recherche sur la Nature et les Technologies and computing resources were provided by the Laboratory of numerical cartography and photogrammetry of the GSC Québec office. The authors would also like to thank Dr. Alfonso Rivera, Dr. Yves Michaud, Valérie Murat and Daniel Paradis for helpful discussions. Dr. Christine Rivard provided a constructive review of the paper. GSC contribution #2004043.

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