VALIDATION OF THE HYDROGEOSPHERE CODE TO SIMULATE CONTAMINANT TRANSFERS THROUGH COMPOSITE LINERS WITH A SINGLE HOLE IN THE GEOMEMBRANE

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ABSTRACT
Migration of chloride inorganic contaminants through a single hole in a geomembrane (GMB) in direct contact with a geosynthetic clay liner (GCL) and an adjacent silty sand is simulated using the 3D HydroGeosphere code. The hole in the GMB is 10 mm in diameter and the applied hydraulic heads are 0.3 and 1 m. Numerical Simulations were performed in order to predict contaminants behaviour to reach complete diffusion of a specific concentration of sodium chloride (NaCl) into the GCL and the soil liner and to compare numerical concentrations with experimental values. Obtained results of NaCl concentrations through the GCL and the subsoil were compared to existing results in order to validate the ability of the used code to predict contaminant transfers through a single hole in the GMB by the coupled phenomena of diffusion and advection. Results of numerical simulations of relative concentrations with time are in good agreement with the theoretical curve for advection-diffusion transport. Furthermore, results of simulated contaminant concentrations agree with observed values for diffusion coefficient of $6x10^{-10}$ m^2/s for the soil and $1x10^{-10}$ m^2/s for the GCL when the hydraulic head is 0.3m and $8x10^{-10}$ and $4x10^{-10}$ m^2/s respectively for the soil and GCL for a 1m applied hydraulic head at the hole. The use of the HydroGeosphere code thus seems on the basis of this study to constitute a new potential tool for giving predictions of effluent concentration with time and chloride distribution in the silty sand in contact with the composite liners that prove to be in good agreement with experimental results from previous studies.

• INTRODUCTION

• Composite liners in landfills

Composite liners used at the base of modern landfills often contain a high-density polyethylene (HDPE) geomembrane (GMB) over a geosynthetic clay liner (GCL). This GMB-GCL association is intended to minimize the leakage and transport of contaminants from the landfill to the surrounding environment (i.e., surface and groundwater). Despite special attention regarding manufacturing, transportation, handling, storage and installation, defects in the GMB seem to be unavoidable (Needham et al. 2004; Peggs et al. 2002). They represent preferential flow paths for leachate migration which could reach and pollute the surrounding soil and groundwater. Defects in the GMBs when present could enhance contaminants transport and hence the pollution of the surrounding environment. As indicated by Brown et al. (1987), the flow through a defect in the GMB due to advective transport depends on the contact between the GMB and the underlying medium. According to these authors, if the contact is not perfect, the fluid that has migrated through the defect spreads laterally within the gap (i.e., the interface) between the GMB and the underlying medium. The area covered by this interface flow is called the “wetted area.” Finally, the liquid migrates into and through the underlying medium. This advective transport due to the hydraulic gradient across the liner is coupled with diffusive transport due to a concentration gradient across the liner. It thus seems important to correctly predict the transport of contaminants in the case when the GMB is exhibiting a hole by taking into account the combination of advective and diffusive transport mechanisms. Various cases have been studied in order to quantify the transport of NaCl though GCLs by diffusion and through composite liners by diffusion-advection using experimental and numerical modelling. These studies are detailed in the next sections.

• EXPERIMENTATION OF DIFFUSION OF NaCl THROUGH GCLS

Lake and Rowe (2000) conducted diffusion tests on three different GCLs using NaCl solutions with different concentrations. They reported that the diffusion coefficient of GCL using NaCl solutions decreased linearly with the decrease in the final void ratio using solution concentrations from 0.05 to 0.08 mol/L NaCl. They also concluded that the type of diffusion test had no effect on the value of the diffusion coefficient. For the sodium bentonite examined, it was reported that the diffusion coefficient of chloride ranged from 1.3×10^{-10} to 3.5×10^{-10}

m^2/s with an average of 2×10^{-10} m^2/s; while the diffusion coefficient of sodium ranged from 6×10^{-11} to 2.5×10^{-10} m^2/s, with an average of 3.4×10^{-10} m^2/s at a source concentration of 3300 mg/L (0.06 mol/L NaCl) when the void ratio ranged from 1.1 to 2. Rowe et al. (2000) performed tests to obtain the inorganic diffusion coefficient of GCLs. They reported that the diffusion coefficients deduced for Na^+ and Cl^- are directly related to the final bentonite bulk ratio.

They also showed that good results could be obtained by modelling the diffusion through the GCL using the bulk porous media diffusion coefficient Dp (Dp = nt Dt, where nt and Dt are the total GCL porosity and the diffusion coefficient, respectively). Lake and Rowe (2000) and Rowe et al. (2000) highlights will be used in the contaminant transport modelling discussed later.

- EXPERIMENTATION OF DIFFUSION OF NaCl THROUGH COMPOSITE LINERS

Rowe and Abdelatty (2013) conducted laboratory experiments to examine the leakage and transport of the 0.14-M NaCl (5,000 mg/L chloride) solution through a composite liner system composed of a 1.5-mm-thick HDPE GMB with a 0.01 m diameter hole (0.785 cm^2) in direct contact with a GCL. The experiments were conducted using a GCL with sodium bentonite and a non-woven cover geotextile in direct contact with the GMB at an applied vertical pressure of about 100 kPa for 0.3 and 1 m hydraulic heads. In these experiments the initial permeant was DW for the first 280 days. This was replaced by a 0.04-M NaCl (1,500-mg/L chloride) solution for 120 days then replaced by a 0.14-M NaCl (5,000-mg/L chloride) solution for the remaining 800 days. The evolution with time of the observed chloride distribution in the silty sand at the end of the experiments was reported at different radial distances and a vertical distance of 0.3 m from the hole. An analysis of the subgrade specimens taken at various distances from the hole and at various depths showed that the contaminant spread around the hole such that a highest concentration was found at the center of the cell and reduced with the radial distance. The contaminant plume was larger than the wetted area, which suggests that the advective-diffusive transport in the silty sand controls the contaminant distribution in the sand. There was also a very significant effect of the head on the distribution of contaminant in terms of concentration.

- NUMERICAL MODELLING OF DIFFUSION OF NaCl THROUGH COMPOSITE LINERS

Rowe and Abdelatty (2012) performed numerical modelling of NaCl contaminants transport through a single hole in the GMB as part of a composite liner following an indirect coupling. In fact, these authors used the axisymmetric finite element flow software SEEP/w to model the steady state flow, and generate Darcy's velocities at the first stage. They then used the finite element software CTRAN/w to model the contaminant transport at the second stage. Numerical simulations of contaminants transport performed by Rowe and Abdelatty (2012) gave very encouraging agreement with the observed migration and distribution of a 0.14 mol/L NaCl solution through a hole in the GMB forming part of a composite liner (Rowe and Abdelatty 2013).

The aim of this paper is to perform and validate numerical modelling of advective-diffusive NaCl transport through GMB-GCL-CCL composite liners using the HydroGeosphere code (Therrien and Sudicky 1996). The choice of HydroGeosphere code was made in relation with its ability to perform direct coupling of advective and diffusive transport of contaminants. Results of contaminants concentrations across the liner will be compared with existing experimental results in the literature (Rowe and Abdellaty 2013) by varying the diffusion coefficient across the liner. This validation of the use HydroGeosphere will allow to further quantify contaminant plume for various contaminants (organic and inorganic) and various situations (hydraulic head, barrier component, etc).

- THE HYDROGEOSPHERE CODE

The HydroGeosphere code (Therrien and Sudicky, 1996) is used for all simulations presented in this paper. It is a 3D control-volume finite element model that simulates variably-saturated subsurface flow and advective-dispersive mass transport in discretely-fractured or unfractured porous media. Like most existing numerical software packages, this code considers that the porous media is incompressible and variably-saturated flow is described by a modified form of Richards' equation, where the storage term is expanded to consider water and soil compressibility (Falaknaz et al., 2015). HydroGeosphere uses a globally-implicit approach to simultaneously solve the 2D diffusive-wave equation and the 3D form of Richards' equation.

For each time step, the model solves surface and subsurface flow, mass and energy transport equations simultaneously and provides complete water balance and solute budgets. The conservative modelling approach fully couples the surface flow and transport equations with the 3-D variably-saturated subsurface flow and transport equations. This approach is significantly more robust than previous conjunctive approaches that rely on linkage of separate surface and subsurface modelling codes (Therrien and Sudicky, 1996).

For solute transport, the model assumes linear equilibrium sorption that is independent of the sorption capacity of the medium, the flow velocity, or the solute residence time. Sorption is described by a retardation factor for the fracture (R_f) and for the matrix (R), respectively. The effective diffusion coefficient for solutes in the matrix is given by the product of the free water diffusion coefficient by the tortuosity. HydroGeosphere can conduct rapid simulations with relatively short computing times and high results efficacy. For most reactive and non-reactive contaminants, the main modes of transport are advection and hydrodynamic dispersion (which includes molecular diffusion and mechanical dispersion). Advection controls the migration by water flow in response to a hydraulic gradient. Mechanical dispersion is the process of contaminants migration due to a concentration gradient, and it takes into account the tortuosity of the medium.

- GENERAL FEATURES OF COMPOSITE LINERS

- Porous media caracteristics

The studied 2D axisymmetric model is shown in Figure 1. It consists of a composite liner formed by a damaged GMB stacked on a 0.01-m-thick GCL overlying a 0.3 m thick silty sand. This scheme is consistent with composite liners used in experiments involving transmissivity cells (Rowe and Abdelatty, 2013). The system was inverted to allow upward flow (from the bottom to the top) of the cell to maximize saturation of the silty sand layer and minimize the risk of trapped air in the system. Thus, the GMB with the hole is at the bottom with the GCL above convered by the silty sand (Rowe and Abdellaty, 2012). A uniform mesh is adopted with 2 $x10^{-03}$ m elements in x direction and 1 $x10^{-03}$ m elements in the vertical direction which have generated a total number of 45 000 elements. The interface between the GMB and the GCL is modeled as a thin layer 0.001 m thick and the hydraulic conductivity was adjusted to give the required transmissivity (Touze-Foltz et al., 2016). Therefore, a uniform transmissivity for the interface equal to $1.1x10^{-7}$ m^2/s according to Rowe and Abdellaty (2012) will correspond to a saturated hydraulic conductivity equal to $1.1x10^{-11}$ m/s.

In addition to groundwater velocity, which is controlled by the porosity of the soil (here silty sand, n = 0.33) and the Darcy flux, contaminant transport will be influenced by the coefficient of hydrodynamic dispersion D. The latter has two components: diffusion and mechanical dispersion. Using the HydroGeopshere code, it is possible to specify the value of the free diffusion coefficient D_0 and the tortuosity τ. The code will calculate the diffusion coefficient D_e for each layer ($D_e = D_0 * \tau$). The features of the porous media are presented in Table 1 and Table 2.

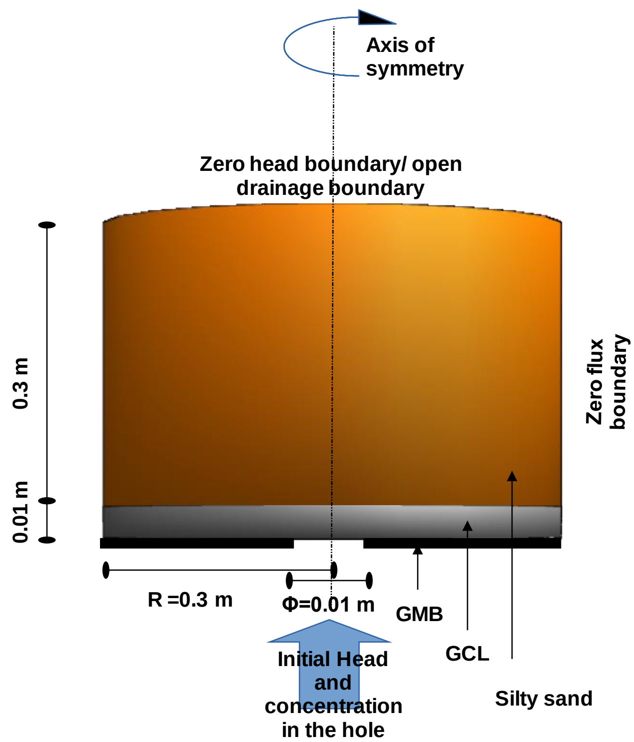

Figure 1. Features of GMB-GCL composite liner (adapted from Rowe and Abdellaty 2012).

Table 1. Parameters of the different porous media

Porous media	Thickness (m)	Porosity (n)	Saturated hydraulic conductivity Ksat (m/s)
Silty sand	0.3	0.33	$1x10^{-6}$
GCL	0.01	0.78	$3.2x10^{-10}$
Interface	0.001	/	$1.1x10^{-8}$

Table 2 Diffusion coefficient and tortuosity values for contaminant transport

Case	Free diffusion coefficient D_0 (m^2/s)	Tortuosity for soil	Tortuosity for GCL	Diffusion coefficient De (m^2/s) for soil	Diffusion coefficient De (m^2/s) for GCL
Case 1	$10x10^{-9}$	0.2	0.1	$2.0x10^{-10}$	$1.0x10^{-10}$
Case 2	$10x10^{-9}$	0.8	0.1	$8.0x10^{-10}$	$1.0x10^{-10}$
Case 3	$10x10^{-9}$	0.2	0.4	$2.0x10^{-10}$	$4.0x10^{-10}$
Case 4	$10x10^{-9}$	0.8	0.4	$8.0x10^{-10}$	$4.0x10^{-10}$
Case 5	$10x10^{-9}$	0.6	0.2	$6.0x10^{-10}$	$2.0x10^{-10}$
Case 6	$10x10^{-9}$	0.6	0.1	$6.0x10^{-10}$	$1.0x10^{-10}$

- Initial and boundary conditions

To simulate contaminant transport by advection-diffusion, a free-drainage boundary condition was used for the bottom boundary, and a no-flow boundary condition was used for the GMB. The GMB is exhibiting a 0.01 m diameter hole. The hole was modeled as a 0.3 m and a 1 m hydraulic head boundary condition respectively. To simulate contaminant diffusion an initial concentration C_0 (Dirichlet or first type) boundary condition was imposed at all nodes of the hole. These simulated initial conditions have already been adopted and confirmed by previous results existing in the literature for inorganic contaminants (Rowe and Abdellaty, 2012). The initial concentration is imposed null elsewhere in the model which will create a concentration gradient across the liner. The intact GMB, side boundaries, and axis of symmetry were zero flux boundary conditions. A no-flow boundary condition was also imposed at the left and right boundaries of the model. A variable grid was adopted by the HydroGeosphere code for the simulated model (x from -0.3 m to +0.3 m and y from 0 to 0.311 m) with variable size elements in x and in y directions. This simulation generated a total number of 34 932 nodes and 17202 elements.

- RESULTS AND DISCUSSION

- Diffusion results at x = 0.134 m (A1)

Figure 2 and Figure 3 show the simulated relative contaminant concentrations C/C_0 for respectively hydraulic heads of h_1 = 0.3m and h_2 = 1m in comparison with experimental results from Rowe and Abdelatty (2013). Relative contaminant concentration values were extracted at an observation well located at x = 0.134 m which corresponds to the receptor zone called A1 in Rowe and Abdellaty (2013)'s experimental work. Relative contaminant concentrations were simulated for a maximum time step of 1000 days (24000 hours). When using the HydroGeosphere code, it is possible to obtain the relative concentration C/C_0 (between 0 and 1) with time.

It can be noticed that simulated and experimental contaminant curves reproduce the theoretical evolution for contaminant transport (Figure 2 and 3).

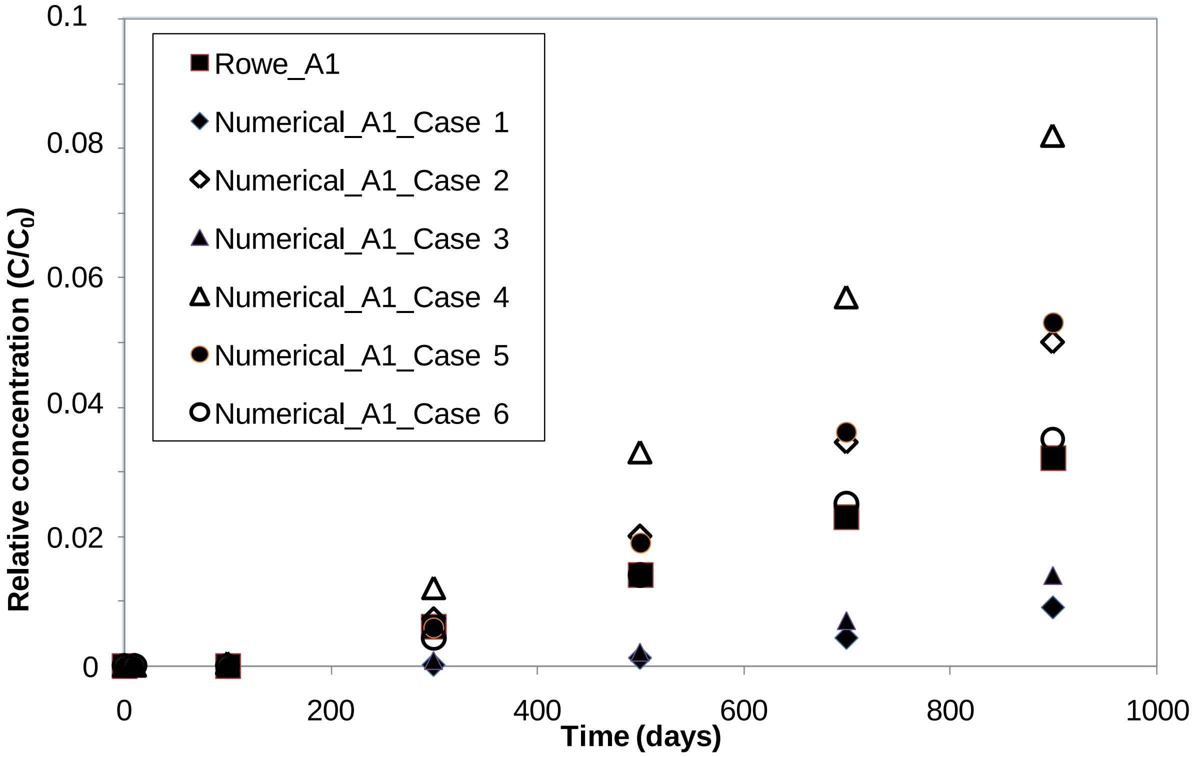

Figure 2. Relative concentration C/C_0 over time for chloride effluent and $h_1 = 0.3$ m; comparison between observed and numerical values at x = 0.134 m (A1) and for various diffusion coefficients.

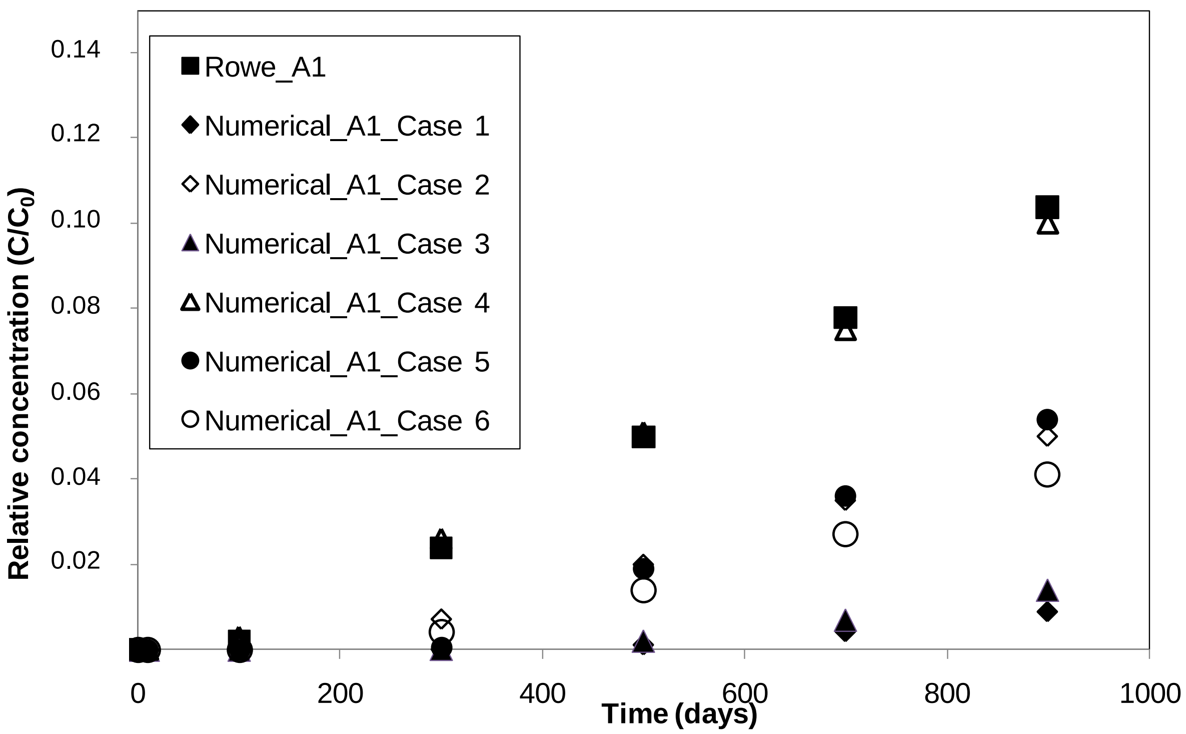

Figure 3. Relative concentration C/C_0 over time for chloride effluent and for $h_2 = 1$ m; comparison between observed and numerical values at x = 0.134 m (A1) and for various diffusion coefficients.

• Diffusion results at x=0.3 m (A5)

Contaminant concentrations were also simulated at the top of the silty sand at x = 0.3 m at the corner of the model by extracting results concentrations from an observation well at x = 0.3 m which corresponds to the receptor zone called A5 in Rowe and Abdellaty's (2013) experimental work. The same concluding remarks could be noticed as for the case of A1. Generally, we conclude that relative contaminant concentrations are lower when moving away from the hole (source of contamination) for both hydraulic heads.

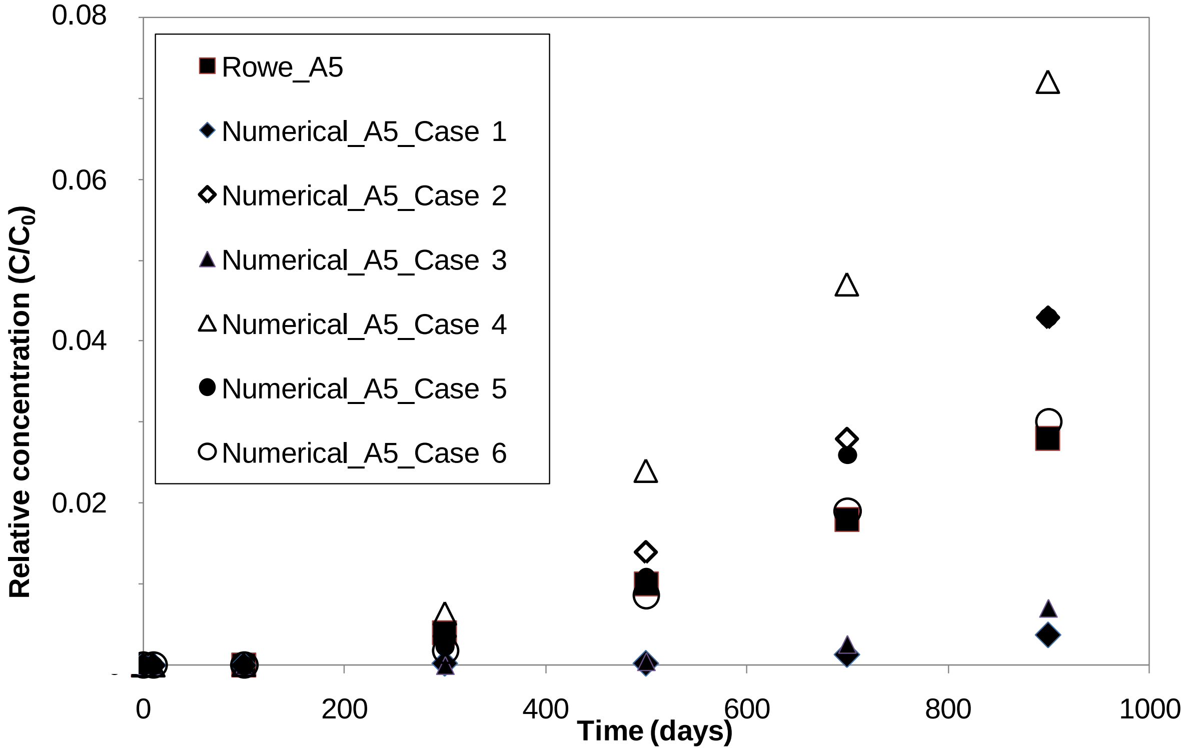

Figure 4. Relative concentration C/C_0 over time for chloride effluent and for h_1 = 0.3 m; comparison between observed and numerical values at x = 0.3 m (A5) and for various diffusion coefficients

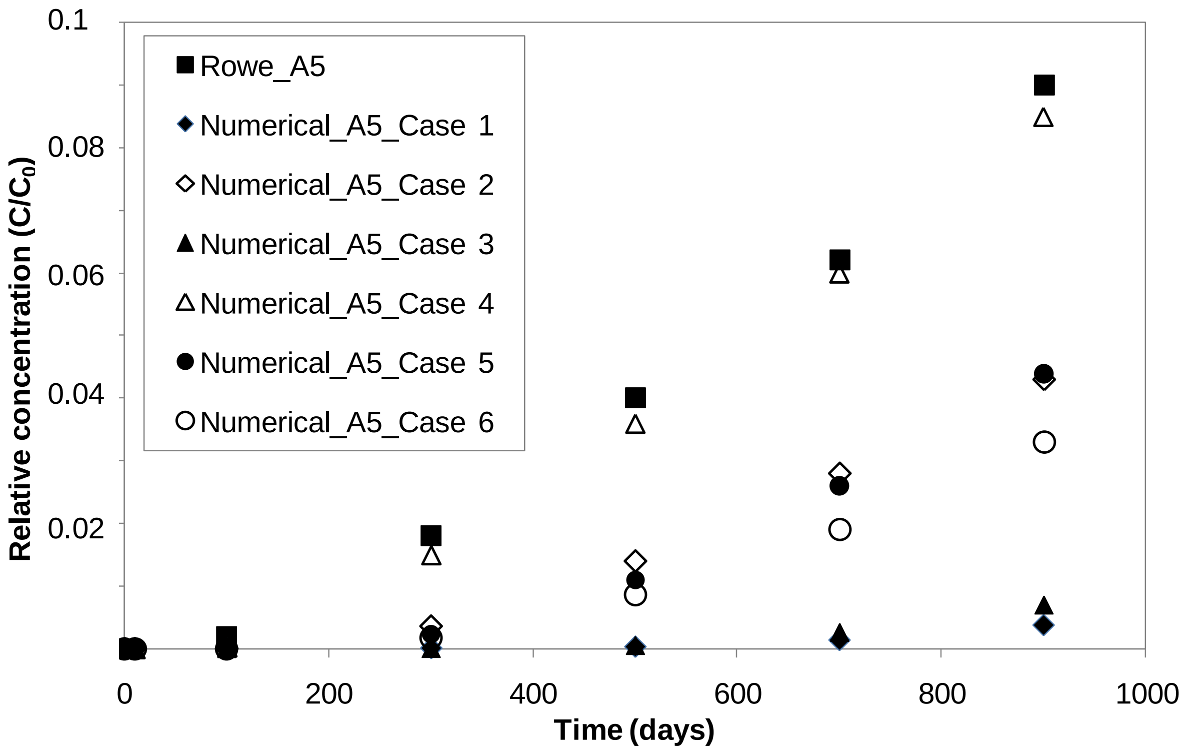

Figure 5. Relative concentration C/C_0 over time for chloride effluent and for h_2 = 1m; comparison between observed and numerical values at x = 0.3 m (A5) and for various diffusion coefficients

Figures 2, 3, 4 and 5 show obtained results of simulated concentrations for six different cases (case 1 to case 6) corresponding to the different diffusion coefficients used (see Table 2) and for two hydraulic heads imposed at the hole (0.3m and 1m). Results show that for all studied cases, a representative shape of the theoretical breakthrough curve of contaminants transport by advection-hydrodynamic dispersion was obtained. Moreover, in these figures, experimental values are also plotted (Rowe and Abdellaty, 2013) in order to compare experiments with simulations. For each case, simulated values were fitted to observed concentrations in order to determine the best values of diffusion coefficients of chloride. For the A1 zone and for a hydraulic head equal to 0.3m, the difference between simulated concentrations and observed values diminishes with time from $4x10^{-1}$ to $8.5\ x10^{-2}$. For the case of a 1m of imposed hydraulic head, the difference between numerical and experimental values also decreases with time from $3x10^{-1}$ to $4x10^{-2}$, and this for the A1 zone.

In reference to Figures 2 and 4 (hydraulic head equal to 0.3m) it can be concluded that the best fit between observed values and simulated concentrations was for case 6 of tortuosity, hence diffusion coefficients of $6x10^{-10}$ and $1x10^{-10}$ m^2/s, respectively for the soil and the GCL. When the applied hydraulic head at the hole is 1m as shown by Figures 3 and 5, the best fit between observed values and simulated concentrations is obtained for case 4 of tortuosity which corresponds to diffusion coefficients of $6\ x10^{-10}$ and $1\ x\ 10^{-10}$ m^2/s, respectively for the soil and the GCL.

In conclusion, when the hydraulic head applied at the hole is increased from 0.3m to 1m, contaminants concentration are more important and contaminants could travel larger distances. In addition, we could notice that in all cases, relative contaminant concentrations remain at lower values and never reach the maximum value imposed at the source. This demonstrates the efficiency of the composite liner.

These results can be explained by the fact that when the hydraulic head increases at the simulated hole in the GM, and for elevated values of diffusion coefficients, contaminants can migrate more rapidly and can travel distances. The results obtained with the HydroGeosphere code also illustrate the influence of the diffusion coefficient on contaminants behaviour and concentrations.

- CONCLUSION

The transport of NaCl through a GMB-GCL-CCL composite liner was simulated using the Hydrogeosphere code. Two different hydraulic heads (0.3 m and 1m) were adopted and two locations in the composite liner were chosen to compare the relative contaminant concentration (A1; A5 from the top of the silty sand) between experimental and numerical data. Results from simulation were compared to previous experimental results in order to validate the use of HydroGeosphere for predicting contaminant transfers through a single hole in the GMB and this for different diffusion coefficients of soil and GCL to obtain the best fit with observed values. Results from this paper have shown that the results obtained with the HydroGeopshere code are in good agreement with previous experimental results for all cases studied with respect to the theoretical behavior of contaminant transfers. In addition, it could be noticed that the increase in the hydraulic head leads to the increase of the NaCl concentration for the same time. Other cases could be simulated to improve these results for other situation and different contaminants.

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