Hydrogeologic modelling for permeable reactive barriers design

Marion Kimmel, Benjamin Piel, Hafid Baroudi, Annette Esnault-Filet, Xavier Laloum, Dominique Mazzieri

HAL Id: ineris-00972419

https://ineris.hal.science/ineris-00972419

Submitted on 3 Apr 2014

HYDROGEOLOGIC MODELLING FOR PERMEABLE REACTIVE BARRIERS DESIGN

Marion Kimmel *, Benjamin Piel *, Hafid Baroudi *, Annette Esnault-Filet **, Xavier Laloum **, Dominique Mazzieri **

* : INERIS, Parc technologique Alata – BP 2, 60550 Verneuil-en-Halatte, France
Phone :   00 33 3 44 55 65 07   Fax :   00 33 3 44 55 65 56
Marion.Kimmel@ineris.fr, benjamin.piel@caramail.fr, Hafid.Baroudi@ineris.fr

** : SOLETANCHE BACHY, 6 rue de Watford, 92000 Nanterre, France
Phone :   00 33 1 47 76 42 62   Fax :   00 33 1 49 06 97 34
aesnault.filet@soletanche-bachy.com, Xavier.Laloum@soletanche-bachy.com,
Dominique.Mazzieri@soletanche-bachy.com

Key words : reactive barriers, groundwater clean-up, in-situ remediation, design method, hydrogeologic modelling

Summary

Permeable Reactive Barrier is an in-situ reactive system used for passive groundwater treatment. The objective of the study performed is the understanding of the hydraulic mechanisms that govern the working of these systems, by the mean of numeric tools for different configurations of sites or contaminations. The study comprises the development of simplified tools such as design charts and the definition of a PRB design methodology. The studied configurations were based on the special patented drain panel® process.

1. Introduction

Permeable reactive barriers (PRB) are passive and in-situ systems for groundwater treatment. Reactive material is placed in the subsurface to intercept a plume of contaminated groundwater moving through the system under its natural gradient. This creates a passive treatment system. Field-scale installation of a reactive barrier requires careful design based on the site-specific hydrogeology and on contaminant plume characteristics. Important parameters to take into account when designing reactive barriers are essentially its position with regard to the contaminant plume, the hydraulic site characteristics, the characteristics of the gate (type of reactive material, geometry), and the depth of the substratum into which the barrier is "keyed". Groundwater flow modelling is a useful tool to understand the hydraulic behaviour of the site and to optimise the reactive barrier design.

The study, conducted by INERIS for SOLETANCHE BACHY, aimed at understanding hydraulic mechanisms by numeric tools, for various types of contamination and site configurations. It also consisted of the development of design tools. Both the creation of simplified tools such as design charts and definition of a PRB design methodology were undertaken. So-called "funnel-and-gate" configurations were studied, implemented by a special patented drain panel® process, with reactive-material filled filters placed in one or several gates, between impervious vertical walls, such as slurry walls.

The first part of the study includes parametric tests. Indeed, the system, although simple in its principle, requires consideration of numerous parameters :

- **the flow rate to channel towards the reactive gates** : it depends on the position and the width of the contamination source, as well as on the hydrogeologic parameters of the site : hydraulic conductivity, transmissivity, pressure head, hydraulic gradient and its seasonal variations.

- **the hydraulic characteristics of the filters** : the pressure head needed to reach a sufficient flow rate depends on the number of filters, their section and permeability. On the other hand, the finer the grain size is, the longer the residence time is.

- **the life-time of the filters** : it depends on the flow rate through the filter, on the retention capacity of the filtering material on the evolution of the contaminant concentrations in the aquifer, and therefore, on the kinematics of exchange between the source of contamination and the groundwater.

- **the dimension of the slurry walls** : because of the pressure head necessary to maintain a sufficient flow rate, the water will be slightly under pressure on the upstream side of the barrier, and some stream lines will move around the system. The higher the pressure head required, the longer the slurry wall must be.

The understanding of these mechanisms and their interactions is the principal object of the study. Numerous models using MODFLOW / MT3D / MODPATH were constructed to simulate the behaviour of the barriers under several configurations of contaminations and site. For each configuration, the sensitive properties were identified and integrated into the design method.

The second part is the development of design tools, using results from the previous simulations. A design method was set up, which allows the determination of both wall and filter lengths, knowing the width of water that moves through the gate(s) (called capture zone), the filter section, and the permeability of the filters and of the aquifer. It was shown that the hydraulic gradient of the site has no impact on the width of the capture zone (if all the other parameters remain equal). The method also allows prediction of the flow rate in the gate(s), and the residence time in the filters.

2. Characteristics of the models used for the development of the design method of the PRB

2.1. Geometry of the models used

Dimensions of the models used for the development of the design method of the reactive barriers are shown in Figure 1. It corresponds to a square, 1000 m wide, 20 m thick.
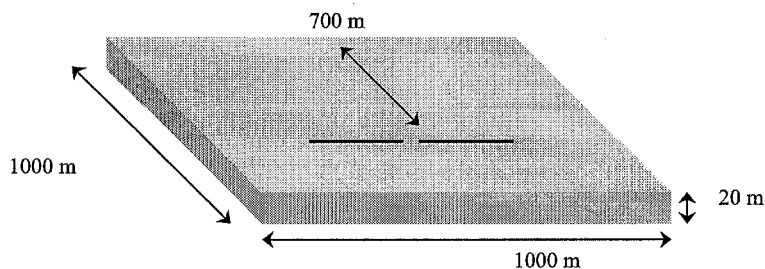

Figure 1 - Geometry of the models

The type of barrier studied here is composed of two watertight walls, of equal length, placed on either side of a gate holding the filtering system. The reactive barrier is placed at 700 m from the upstream limit of the model, because the impact of the barrier is higher upstream than downstream.

The boundary conditions are set equal to the following parameters :

- upstream and downstream constant hydraulic heads, respectively 20 and 15 meters.

- side and base limits : it corresponds to no-flow limits.

The hydraulic gradient, which results from the former boundary conditions, is 5.10^{-3}. A high gradient was selected so as to contrast the flows which circulate in the reactive gate of the barrier. The height of water, at the location of the filters, reaches 17 m. The hydraulic conductivity of the aquifer lies between 10^{-6} and 10^{-3} m/s.

2.2. Presentation of the drain panel®, and modelling of the filter system

The drain panel® system allows for the installation of a battery of multiple removable filters, filled by reactive materials. This system was developed and patented by SOLETANCHE BACHY. The construction principle is illustrated in Figures 2 and 3.
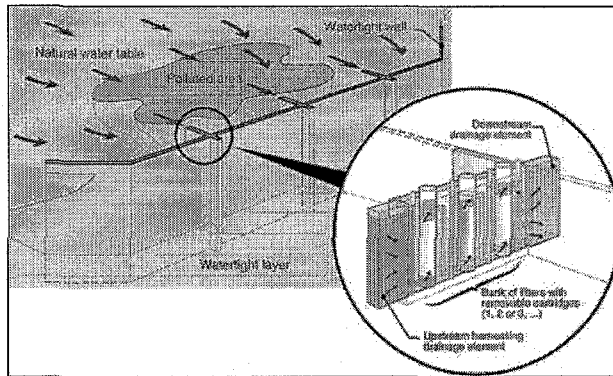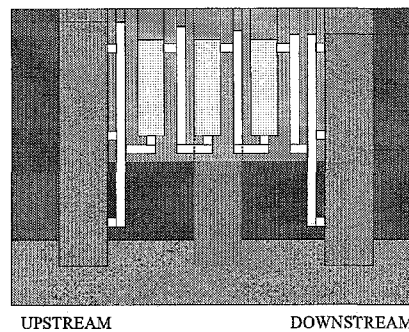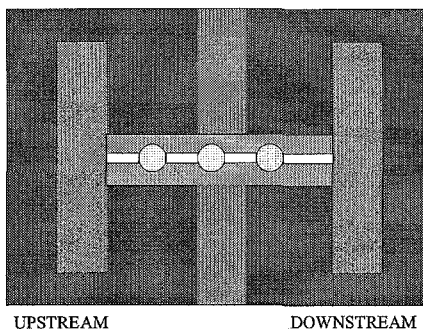
Figure 2 - Principle of the drain panel® (developed and patented by SOLETANCHE BACHY)

UPSTREAM   DOWNSTREAM   UPSTREAM   DOWNSTREAM

Figures 3a and 3b - Top view and cross-section of the drain panel®

The aquifer is represented by the brown colour, upstream and downstream piezometric levels are shown on figure 3b. The various elements of the device to model are the following :

- Watertight barrier : (in dark grey) Its width is 0,60 m, it is keyed in a impervious substratum.

- Slurry wall : (in clear grey) Its width is 0,60 or 1,2 m according to the size of the filters, its length is 2,50 m.

- Upstream and downstream drains : (sandy colour) Their width is 0,60 m. Their length is variable. Their hydraulic conductivity ranges between 10^{-2} and 1 m/s.

- Filters : (in yellow) Two diameters are used : 0,40 m (for a gate width of 0,60 m) and 0,90 m (for a gate width of 1,2 m). 1, 2 or 3 filters are used, of unit length 3 meters, Their permeability varies from 10^{-4} to 10^{-2} m/s, depending upon the nature of the reactive material, its state of compactness and clogging.

- Pipes : (in white when it is filled with water, transparent in the other case)

To be modelled under MODFLOW, the drain panel® must be compared to a simpler structure. The purpose of the following calculation is to simplify the geometry of the device, according to the following diagram (figure 4) :
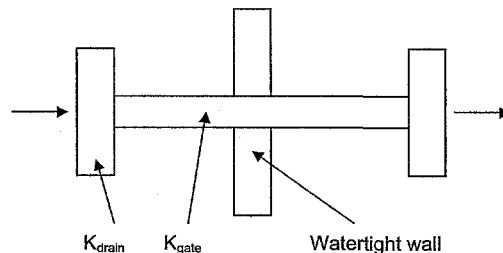

K_{drain} K_{gate} Watertight wall

Figure 4 - Principle adopted to model the reactive gate and the drains

For the needs of the modelling, the gate becomes a parallelepiped filled with reactive material.

The filters are the elements governing the flow through the device. The calculation that follows makes the assumption that the pressure losses in the pipes are negligible, and only takes into account the pressure losses in the filters.

The system is compared to several filters, with a length L, placed end to end as shown in figure 5 :

Figure 5 - Principle adopted to group the filters for the needs of calculation

The flow that circulates through the gate is calculated by the following formula, obtained from Darcy's law :

$$Q = K_f . \frac{\Delta P}{n_f . L} . S_f$$

with : K_f = hydraulic conductivity of the filter $\qquad$ ΔP = total pressure losses in the filters
n_f = number of filters $\qquad$ L = length of a filter
S_f = section of the filters = Π (D / 2)² $\qquad$ D = diameter of the filters

By simplifying the geometry of the gate, in order to obtain a right-angled parallelepiped filled by reactive material of equivalent permeability, the flow equals to :

$$Q = K_e . \frac{\Delta P}{2,50} . h.l$$

with: K_e = equivalent permeability of the gate $\qquad$ 2,50 m = length of the gate
h = height of water in the aquifer $\qquad$ l = width of the gate in the model (0,60 or 1,20 m)

$$\text{so} : K_e = \frac{K_f}{n_f L} . \pi \left(\frac{D}{2} \right)^2 \frac{2,50}{h.l}$$

The models are discretized in a grid that includes between 40 000 and 47 000 cells depending on the length of the slurry walls. Grid-cells measure 20 m as a maximum, apart from the zone where the barrier is set. The cell size decreases regularly along the barrier, in direction of the filter gate, from 8,4 to 0,2 m. The reactive gate is discretized as shown in figure 6 : the gate, which measures 0,60 m or 1,20 m according to the diameter of filter chosen, includes 4 cells in its width. Models were carried out in order to test the discretization sensitivity. The model for a gate of 0,60 m width included 2 or 6 cells to represent the gate width. The values of flow in the gate were different from 0,4 %. The option with 4 cells, rather than 2, was selected because it allowed better simulations of trajectories under MODPATH.
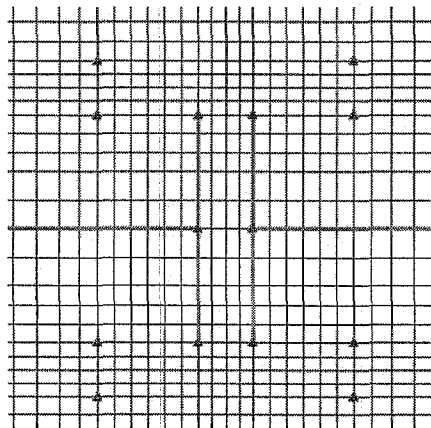

Figure 6 - Mesh used to model the filtering gate

3. Development and presentation of the design method of the PRBs

3.1. Sensitivity analysis of the parameters

Works of Starr & Cherry (1994) and Teutsch & al. (1997) specify that, in the case of simple reactive barriers (without drain and reagent, simply established in a trench), only the width of the gate, the length of the slurry walls and the relationship between the transmissivity of the gate and the transmissivity of the aquifer, govern the width of the capture zone. Thus, according to these authors, the hydraulic gradient has no influence over the width of the capture zone. Validity of this assumption was checked when applied to drain-panel system. Lastly, according to the works of Starr & Cherry (1994), the flow in the gate is maximum for an angle of barrier of 180°, and for watertight walls placed at 90° of the direction of the regional flow. This configuration was the only one taken into account in the models.

3.2. Steps of the design method

The basic idea retained for the design method of PRB consists in determining the capture zone width (the width of the water band of the aquifer) which has to circulate through the reactive gate (figure 7). Then, according to the characteristics of the aquifer, and to the filters chosen, the second stage consists in determining, by the use of design charts, the length of watertight wall necessary for the desired capture zone. If the design charts do not allow it, some design methods for drains or additional gates are then proposed.

The design of a permeable reactive barrier proceeds according to the following steps :

❶ Calculation of the future flow rate through the gate

The designer must know several parameters characterising the reactive barrier site location :

♦ the local hydraulic gradient of the site, i ;   ♦ the height of water in the aquifer, h ;

♦ the hydraulic conductivity of the aquifer, K_{aq} ;   ♦ the width of the contamination plume, Z_c.

The capture zone, Z_c, concretely corresponds to the lateral extent (in the direction perpendicular to the groundwater flow) of the contamination plume, where the contaminant concentrations are higher than the acceptable standard, calculated either with or without a safety factor. See figure 7.
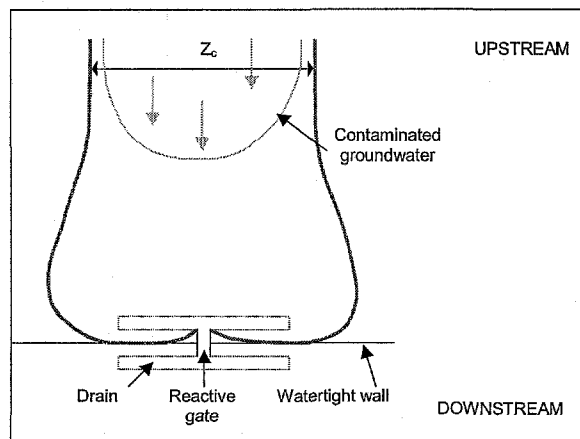

Figure 7 – Z_c definition

By a calculation using Darcy's Law, the user determines the water flow which circulates in the portion of aquifer limited by Z_c and thus through the gate of the future barrier :

$$Q = K_{aq}.Z_c.h.i$$

❷ Choice of the drain panel® equipment

The user has to choose the characteristics of the filters : diameter and hydraulic conductivity K_f. The hydraulic conductivity of the filters will be a function of the constitutive material.

For high permeabilities of aquifer (10^{-4} m/s), it is recommended to use filters of 0,9 m in diameter, which are able to accommodate larger flows.

❸ Calculation of the filter length

The length is calculated using the following criteria :

1. The life-time of the system has to be sufficient : knowing the quantity of contaminant which can be sorbed per g of reactive material, and the concentration in the inlet of the gate, the designer is able to estimate the quantity of reactive material necessary to obtain an acceptable renewal time for the filters.

2. The transit time in the filters has to be sufficient to achieve a satisfactory treatment, even at the end of the life-time of filters.

❹ Determination of the length of the barrier

The designer, knowing the width of the contamination plume (that is the capture zone) and the length of filter to be used, can calculate the length of watertight barrier that is needed to obtain the desired flow through the gate. To achieve that, he needs to choose and use the design chart corresponding to the hydraulic conductivity of the aquifer and his filters, as well as the filter diameter . Figure 8 is an example of design chart relating the zone of capture, the total length of filter, and the length of the watertight walls.
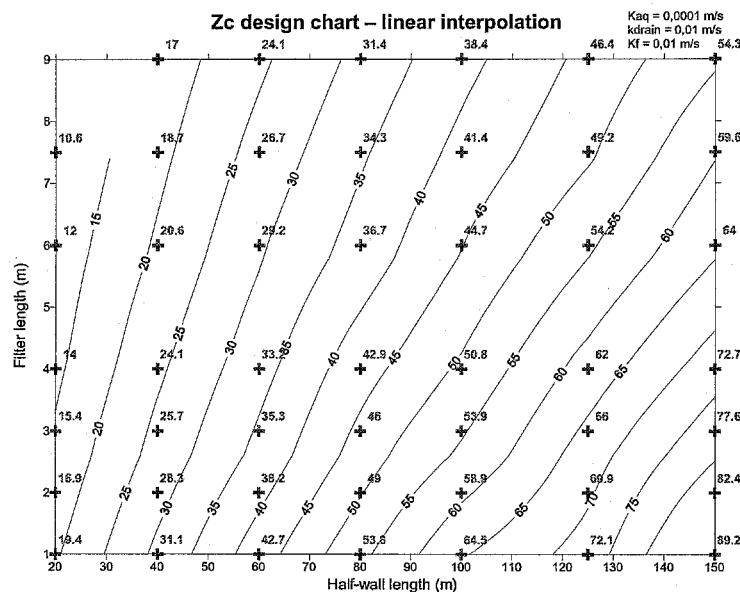

Figure 8 - Example of design chart relating the capture zone, the filter length, and the watertight walls length

The design charts were drawn by simulating various aquifer and barrier configurations (watertight walls lengths, filter lengths, drains and aquifer hydraulic conductivities, and gate widths)..

Design charts are not suited for the following conditions : if the capture zone is too narrow (< 10 m) or if the water flow in the gate is too low (< 1 m³/day), which constitutes an instability factor for the simulations.

General deductions were drawn, thanks to the development of these design charts :

-   A high aquifer hydraulic conductivity causes a high water flow through the gate, but a narrow extended capture zone.

-   A small length of filter induces weak pressure losses, resulting in a high water flow through the gate, and a broad capture zone.

-   A low filter hydraulic conductivity decreases the water flows and the capture zones.

-   For $K_{aq} = 10^{-4}$ m/s, a value of $K_f \geq 10^{-3}$ m/s is necessary to obtain a sufficient capture zone.

- The design charts are identical, whatever the drain hydraulic conductivity is (for the same K_{aq} and K_f).

Two aquifer hydraulic conductivities were definitely isolated from the design method, for hydraulic reasons : the aquifer hydraulic conductivity 10^{-3} m/s generates too high water flows through the gate for very small capture zones. On the contrary, the aquifer hydraulic conductivity 10^{-6} m/s generates very broad capture zones and low water flows through the gate. These cases were not developed further . The design charts corresponding to the aquifer hydraulic conductivity 10^{-3} m/s are nevertheless available.

The design charts were calculated for a drain length of 2,8 m and a water height in the aquifer of 17 m. If the water height in the aquifer is lower than 17 m, the barrier designer can apply corrective coefficients to the capture zone, indexed in tables such as that presented on figure 9. These coefficients were also obtained by series of simulations.

Filter length (in m)	Hydraulic conductivity of the filter (in m/s)	Z_c corrective coefficient
1	10^{-2}	1,08
4	10^{-2}	1,3
9	10^{-2}	1,5
1	10^{-3}	1,55
4	10^{-3}	2
9	10^{-3}	2,2

Figure 9 - Corrective factors for a 7-m high watertable (gate 0,6 m, aquifer 10^{-5} m/s)

❺ Determination of the necessary drain length

If the width of the capture zone does not appear in the available design chart, the designer chooses a smaller capture zone and can increase it by referring to tables of increase of drain length. Those correspond to all the configurations of aquifer hydraulic conductivities, lengths of slurry wall and sizes of gate. The designer will take care not to exceed the maximum drain length (in red in the table), to exploit the gates at the maximum of their capacity. Indeed, when the equivalent hydraulic conductivity applied to the gate is too low to let the water flow through the gate, groundwater that flows through the drains, of high permeability, can move around the barrier. The following figure is an example of table containing corrective coefficients of the capture zones according to the drain length, for watertight walls lengths ranging from 2x80 to 2x150 m (gate 0,6 m, aquifer 10^{-5} m/s, filter 10^{-2} m/s)

Drain length (n*2,8 m)	Z_c corrective coefficient		
	Filter length : 1 m	Filter length : 4 m	Filter length : 9 m
5,6 m = 2*2,8 m	1,09	1,07	1,06
8,4 m = 3*2,8 m	1,14	1,12	1,09
11,2 m = 4*2,8 m	1,19	1,16	1,14
28 m = 10*2,8 m	1,42	1,35	1,29
56 m = 20*2,8 m	1,68	1,55	1,43
70 m = 25*2,8 m	1,79	1,64	1,49
140 m = 50*2,8 m	2,19	1,91	1,66
210 m = 75*2,8 m	2,47	2,05	1,70
280 m = 100*2,8 m	2,52	1,93	1,50

Figure 10 – Z_c corrective coefficients if drains are added to the system

The tables mentioned above are adapted to filters of hydraulic conductivity 10^{-2} m/s. However, hydraulic conductivities of filters can be less, either due to the grain size distribution of the filtering materials, or secondary chemical reactions which take place within the filters, such as carbonate precipitation, leading

to an important reduction in K and possible clogging. Corrective coefficients of the capture zone by decreasing the permeability of the filters were calculated and are proposed to the designer in tables like figure 11.

Filter length	1 m	4 m	9 m
Z_c corrective coefficient	0,60	0,35	0,25

Figure 11 - Example of table for the estimation of the capture zone for a filter permeability of 10^{-3} m/s, compared to a filter of 10^{-2} m/s

The tables allow the designer to evaluate the possibilities for contaminated water to move around the reactive barrier, for example in the event of filters clogging.

❻ Multi-gate system design

If the capture zone obtained at the end of the stage ❺ is not satisfactory, the designer can increase the number of gates and begin again the design at the step of his choice : ❹ or ❺. It should not be forgotten to re-evaluate the necessary filter length for each gate. One has to check that the capture zones of the gates do not overlap. If this is the case, the length of the wall between the gates must be increased.

The main objective of the multi-gate system is to split up the desired total capture zone into multiple capture zones of smaller size assigned to several gates. This method allows an identical capture zone to be obtained with reactive filters of lower permeability and higher length. All gates are supposed to be exactly the same : filter properties, drains,...

In general, it appeared during the simulations, that the capture zone of a system with n gates is n times bigger than the capture zone of a system with one gate (same equipment of the barrier). To design the reactive barrier, the capture zone to be assigned to each filter gate must be equal to $Z_{c\,1gate} = Z_c/n$, with n the number of gates of the system.

The multi-gate design begins with the design of a barrier intercepting Z_c/n with a given filter length. The designer uses the adequate design chart and calculates the length of slurry wall necessary to intercept Z_c/n. Let L be the half-length of barrier. Then, the designer compares Z_c/n to L (mono-gate half barrier length) :

- If $Z_c/n < L$ (no overlapping) :

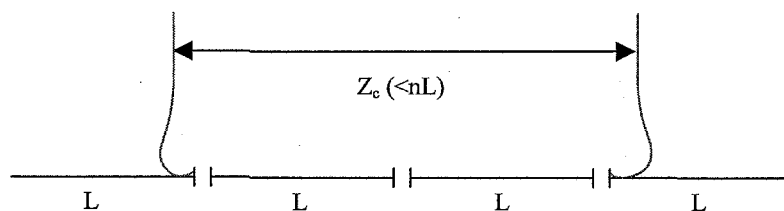In this case, the multi-gate PRB design is :

$$Z_c\ (<nL)$$

L   L   L   L

Figure 12a – Design of multi-gate barrier (n=3) in case of no overlapping.

The total length of the multi-gate barrier is (n+1)L ($>Z_c$).

- If $Z_c/n > L$ (overlapping) :

In this case, where the capture zones of two gates overlap, inter-gate lengths have to be increased and the multi-gate PRB design is :
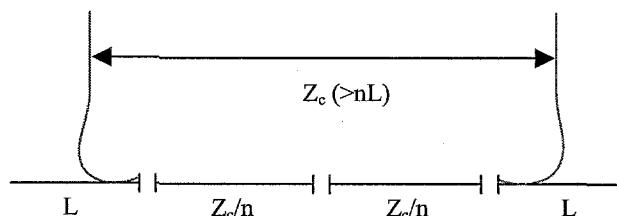

$$Z_c\ (>nL)$$

L Z_c/n Z_c/n L

Figure 12b – Design of multi-gate barrier (n=3) in case of overlapping.

The total length of the multi-gate barrier is $2L + (n-1).Z_c/n$ ($>Z_c$, since the capture zone of a mono-gate system cannot be wider than the barrier ($2L$)).

At the conclusion of steps 4, 5, or 6, the design of the reactive barrier is complete. It is always possible to begin again designing at a former step, in order to have several possible configurations, and in order to make a choice according to the technical and economical constraints of the project.

3. Conclusion

The design method of the PRBs equipped with drain panel[®] system, was conceived by INERIS for SOLETANCHE BACHY using many numerical simulations of barrier installation on simple cases of groundwater flows. The method is organised into 6 steps, which allows, according to the configuration of a contamination plume in groundwater, the design of the reactive filters, the length of the watertight walls and of the drains, and determination of the number of gates.

This method was validated, always using numerical simulations, by modelling real cases. In addition, a prediction method of the contamination migration was conceived using 1-D or 2-D analytical solutions. These solutions allow to predict the evolution of the contaminant concentrations upstream of the reactive barrier, in order to evaluate the life-time of the filters.

References

Gupta, N. & Fox, T.C. (1999) – Hydrogeologic modelling for permeable reactive barriers. Journal of Hazardous Materials 68 ; 19-39.

Starr, R.C. & Cherry, J.A. (1994) – In situ remediation of contaminated groundwater : the funnel-and-gate system. Groundwater 32(3), 465-476.

Teutsch, G., Tolksdorff, J. & Schad, H. (1997) – The Design Of In-Situ Reactive Wall Systems – A Combined Hydraulical-Geochemical-Economical Simulation Study. Land Contamination and Reclamation, 5, No 3, 125-130.