Environmental Science and Pollution Research, September 2018, Volume 25, Issue 27, pp 26793–26800
DOI: 10.1007/s11356-017-0220-y

Discontinuous Permeable Adsorptive Barrier design and cost analysis: a methodological approach to optimisation

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Abstract

The following paper presents a method to optimize a discontinuous permeable adsorptive barrier (PAB-D). This method is based on the comparison of different PAB-D configurations obtained by changing some of the main PAB-D design parameters. In particular, the well diameters, the distance between two consecutive passive wells and the distance between two consecutive well lines were varied, and a cost analysis for each configuration was carried out in order to define the best performing and most cost-effective PAB-D configuration. As case study, a benzene-contaminated aquifer located in an urban area in the north of Naples (Italy) was considered. The PAB-D configuration with a well diameter of 0.8 m resulted the best optimised layout in terms of performance and cost-effectiveness. Moreover, in order to identify the best configuration for the remediation of the aquifer studied, a comparison with a continuous permeable adsorptive barrier (PAB-C) was added. In particular, this showed a 40% reduction of the total remediation costs by using the optimised PAB-D.

Keywords: *permeable adsorptive barrier; benzene; groundwater remediation; adsorption; design and cost analysis; design optimisation.*

1. INTRODUCTION

Groundwater is a fundamental water supply for drinking, agricultural and industrial uses, as highlighted by several authors (Arshad and Imran 2017; Nampak et al. 2014; Venkatramanan et al. 2015). Prevention and protection of groundwater quality from pollution are essential key elements of a proper management of this important natural resource, in order to avoid its depletion and potential negative effects on human health (Li et al. 2017; Wongsanit et al. 2015). For this reason, in recent decades, the scientific community has been focusing on how to remove the numerous existing types of pollutants from groundwater and in particular for micro-pollutants and resistant contaminants (Iovino et al. 2015, 2016; Molino et al. 2013; Musmarra et al. 2016). Permeable Reactive Barriers (PRBs) (U.S. EPA 1999) are an innovative and flexible *in-situ* technology to protect and remediate aquifers from different types of contaminants, e.g. heavy metals (Luo et al. 2016; Park et al. 2012) and organic compounds (Erto et al. 2012; Gao et al. 2015). They are a passive and cost-effective method, which consist of a vertical wall crossing the polluted aquifer. The PRB denomination is because a reactive medium is used to fill the whole barrier, whose hydraulic conductivity is higher than the surrounding aquifer to boost the polluted water to flow through it, by exploiting the aquifer natural gradient (U.S. EPA 1999). The main disadvantage of PRBs are clogging phenomena. If an adsorbing material is adopted as barrier filler, PRBs can be defined as Permeable Adsorptive Barriers (PABs) and the groundwater remediation occurs by adsorption.

In their typical configuration, PABs are a continuous wall (PAB-C); however, several innovative configurations such as discontinuous permeable adsorptive barriers (PABs-D) have been proposed during last few years (Bortone et al. 2013; Wilson et al. 1997). A PAB-D includes an array of passive wells disposed in one or more columns at a given distance from one another and filled with adsorbing materials. Such configuration is more advanced than PAB-C as it allows to remediate the same volume of polluted groundwater with a smaller barrier volume and consequently at a lower cost (Santonastaso et al. 2015).

This paper presents a method for PAB-D optimisation, applied to an aquifer located in north of Naples (Italy), already used as case study in previous papers (Bortone et al. 2013, 2015; Santonastaso et al. 2015). In this site, the presence of both organic and inorganic pollutants was recorded by analytical data deriving from dedicated measurement campaigns. In particular, benzene, which is listed among the priority contaminants by U.S. EPA as carcinogenic (Staples et al. 1985; WHO, 1993), was found at concentrations higher than the Italian regulatory limit (C_{lim}=1 μg L^{-1}) set for groundwater quality. The approach presented is based on testing various PAB-D configurations - all of them allowing for a successful treatment of the contaminated plume - and a successive cost analysis, comparing the layouts obtained with their relative costs, with the aim of minimising the overall remediation cost. The PAB-D array optimization was performed by varying the PAB-D well diameter, and assuming both the distance between two consecutive wells and the distance between two consecutive well lines as function of the well diameter itself. Remediation costs were calculated as a sum of the well drilling costs, the adsorbing material costs and the monitoring well installation costs.

Finally, a comparison between a PAB-C, already designed for the remediation of the same site (Bortone et al. 2015), and the optimized PAB-D configuration was carried out, in order to identify the best and most cost-effective remediation solution.

2. MATERIALS AND METHODS

2.1 Process modelling

The advection-dispersion-reaction equation (Equation 1) can be used to describe the evolution of pollutant species in groundwater over time, when adsorbing phenomena occur, which is written as follows (Bear 1979):

$$\frac{\partial C}{\partial t} = \nabla \cdot (D_h \nabla C) - \frac{\vec{u}\nabla C}{n_s} - \frac{\rho_b}{n_b}\frac{\partial \omega}{\partial t} \quad (1)$$

In Equation 1, C is the groundwater contaminant concentration, t is the time, D_h is the hydrodynamic dispersion tensor, $\vec{u}$ is the water flow rate, n_s is the site porosity, ρ_b is the adsorbing material bulk density, n_b is the barrier porosity and ω is the pollutant concentration on the adsorbent (i.e. its adsorption capacity). The hydrodynamic dispersion tensor, D_h , is expressed as the sum of the tensor of mechanical dispersion, D_m, and the coefficient of molecular diffusion, D_{iff}, (a scalar), as better described by Konikow and Grove (1977). Darcy equation (Equation 2) can be used to evaluate the water flow rate $\vec{u}$ as:

$$\underset{u}{\rightarrow} = K_s \ \nabla C \tag{2}$$

where K_s is the hydraulic conductivity and h is the hydraulic head. The last term on the right side of Equation (1) accounts for PAB adsorption phenomena and can be defined as in the following equation:

$$\frac{\rho_b}{n_b}\frac{\partial \omega}{\partial t} = k_c a\left[C - C^*(\omega)\right] \tag{3}$$

where k_c is the mass transfer coefficient of adsorption, a is the external specific surface area of adsorbent particles and $C^*(\omega)$ is the pollutant concentration in the liquid phase at thermodynamic equilibrium with the concentration on the adsorbent (ω). The thermodynamic equilibrium is usually expressed through an adsorption isotherm, such as the Langmuir model (Equation 4):

$$\omega = \frac{\omega_{\max} K C^*(\omega)}{1 + K C^*(\omega)} \tag{4}$$

where ω_{max} and K are the Langmuir parameter. The computational domain was defined by considering a 2D system, and by assuming constant concentrations of benzene along the vertical groundwater direction and the reference border coinciding with the boundary of the site domain. Moreover, an initial concentration of benzene onto the adsorbing material of the PAB equal to zero and a constant porosity in all computational domain were assigned. The following initial and boundary conditions were used:

$$C = 0 \begin{cases} x = 0 & \forall y \forall t \\ y = 0 & \forall x \forall t \\ y = Y & \forall x \forall t \end{cases} \tag{5}$$
$$\frac{\partial C}{\partial t} + \underset{u}{\rightarrow} \nabla C - \nabla \cdot (D_h \nabla C) = 0 \quad x = X \quad \forall y \forall t$$

X and Y were assumed as coincident with the size of the computational domain, in the x- and y-directions, respectively. A finite element method was adopted to numerically solve the equation system (1)-(4), with the related initial and boundary conditions (5), in COMSOL Multi-physics® environment.

2.2 PAB-D optimization approach

PABs drilling may be a complex task in the case of deep aquifers; adsorptive passive wells (i.e. a PAB-D) can be more appropriate and easier to implement than a PAB-C. Moreover, if a PAB-D is properly designed and strategically placed in a polluted site, it is a very cost-effective technology. In order to minimise PAB-D dimensions and their related costs, a methodological approach to optimize PAB-Ds is proposed in the following. This approach is based on the definition of a set of PAB-D configurations - all allowing for a successful treatment of the polluted plume - which are identified by combining a design optimization technique, previously proposed by the authors (Santonastaso et al. 2015), and a cost analysis for each PAB-D well array layout obtained. As described elsewhere (Bortone et al. 2013, 2015; Santonastaso et al. 2015), to design a Permeable Adsorptive Barrier we required a preliminary field investigation of the area, aimed at describing its hydrogeological characteristics, groundwater hydraulic head and direction, as well as the location, nature and extension of the site contamination. The main objective of a proper PAB-D design is the identification of a geometric configuration of passive wells, permitting the capture of the whole contaminant plume and cleaning the polluted groundwater. The PAB-D geometric parameters are shown in Figure 1 and can be listed in the following as:

- passive well geometrical parameters (such as well diameter (D_w) and well height (H)),
- distance between two consecutive passive wells (I) along a column or line,
- line-to-line distance (d_c),
- number of well lines (n_c) of an array,
- array orientation (ε) and well-barrier position (Bortone et al. 2013; Santonastaso et al. 2015).

As sketched in Figure 1, wells with a squared cross-section were considered. It is worth highlighting that the total number of wells (n_w) depends on D_w, I and d_c. Moreover, an appropriate adsorbing material is required. By varying one of these parameters, such as D_w, I or d_c, a different PAB-D configuration is obtained. In each configuration, the height of wells (H) can be kept constant and equal to the aquifer thickness. In addition, a well array is disposed so that each well line is orthogonal to the groundwater flow direction and as close as possible to the contaminated plume.

Figure 1. Design parameters of a PAB-D (Bortone et al. 2013)

Each PAB-D configuration was determined by varying D_w and assuming that both distance between two consecutive passive wells (I) and line-to-line distance (d_c) were function of the corresponding well diameter. In turn, a variation of D_w, I and d_c results by varying the number of wells (n_w) in each line.

According to the optimized design technique used (Santonastaso et al. 2015), once a PAB-D configuration is set with fixed values respectively for D_w, I and d_c, successive steps aim at determining the number of wells (n_w) for each line and the number of lines of the whole array (n_c). In this way, the minimum total number of wells for each configuration can be assured and, consequently, the minimum amount of adsorbing material, allowing both the capture and the treatment of the pollutant with outlet concentrations lower than the regulatory limit. A heuristic method was used to implement the design optimization technique (Di Nardo et al. 2014).

In addition, a cost analysis was made to assess the remediation cost (C_R) of each configuration. PAB-D drilling costs (C_{well}), adsorbing material costs (C_{Ad}) and monitoring costs (C_M) were considered, while operation and maintenance costs were excluded since PABs are a passive remediation technique, hence they do not need energy consumption and workers. C_R was determined as sum of the costs above written, as shown in Equation 6:

$$C_R = C_{well} + C_{Ad} + C_M \quad (6)$$

The methodological approach was finalized at identifying the most cost-effective PAB-D configuration, among those tested, with the lowest remediation cost, according to the following objective function (O.F.):

$$O.F. = \min\left[C_R\left(D_w, I, d_c\right)\right] \quad (7)$$

3. CASE STUDY

The PAB-D optimization method was applied to the remediation of an aquifer in the surroundings of an urban area located in north of Naples (Italy). In the study area, which is approximately 225 ha, there are numerous solid waste landfills and the underlying aquifer has an average thickness of 8m, with an impermeable layer at a depth of about 40 m from the soil surface. Groundwater soil composition was schematized as a single layer consisting of Neapolitan yellow tuff with hydraulic conductivity (K_S) and longitudinal dispersivity (α_x) equal to 5×10^{-5} m s^{-1} and 1 m, respectively. The equation proposed by Gelhar et al. (1992) was used to estimate transverse dispersivity (α_y):

$$\alpha_y = \alpha_x / 10 \quad (8)$$

Several contaminants, both inorganic and organic, were measured in the aquifer. Among them, benzene was detected at concentrations over 6 times higher than the corresponding Italian regulatory limit for groundwater quality (C_{lim}=1 μg L^{-1}). In Figure 2, the benzene initial concentrations, the groundwater piezometric heads and direction are sketched. The contaminant plume extends for an area of about 500 m x 450 m; the aquifer is east-west oriented with piezometric levels from 12 to 7 m, under a gradient (J) of 0.01 m m^{-1}.

Figure 2. Benzene iso-concentrations and groundwater piezometry of the study area

The main characteristics of the aquifer, including the molecular diffusion coefficient of benzene, are listed in Table 1.

Table 1. Main characteristics of the study area

Adsorption was modelled by using an activated carbon, obtained by H_3PO_4 acid activation of the stems of Arundo Donax, as adsorbing material, which was tested by Basso and Cukierman (2005) for benzene capture from polluted water. The benzene adsorption isotherm is described via the Langmuir model, as expressed by Eq. (4), with ω_{max} and K equal respectively to 35.1 mg g^{-1} and 0.0577 L mg^{-1} (Basso and Cukierman 2005). The main characteristics of the adsorbing material are collected in Table 2. The design optimization was performed on a set of different PAB-D configurations, which were defined by varying D_w in the range between 0.4-1.2 m, while the distance between two consecutive passive wells (I) and the line-to-line distance (d_c) were set equal to twice the diameter and equal to the diameter respectively. The set of configurations tested is summarised in Table 3.

Table 2. Main characteristics of the adsorbing material

Table 3. Set of configurations considered for the design optimization

As already stated, the cost analysis was performed considering the well drilling cost (C_{well}), the adsorbing material cost (C_{Ad}) and the monitoring cost (C_M) for each configuration. The well drilling cost depends on both well diameter and number of wells. The larger the well diameter the higher the well drilling unit cost, expressed per unit of perforation depth; moreover, it depends on the geological soil composition. The adsorbing material unit cost, expressed for unit of volume of adsorbing material, and the monitoring cost were kept constant for all PAB-D configurations. The well drilling unit costs, with feasible drilling diameters, were determined through a preliminary techno-economical survey based on local market indications. The adsorbing material unit cost and monitoring cost were determined through market surveys as well. All well drilling unit costs (C_{well}), the adsorbing material unit cost (C_{Ad}) and the monitoring costs (C_M) considered, are reported in Table 4.

Table 4. PAB-D unit costs

4. RESULTS AND DISCUSSION

The main results obtained for all six PAB-D configurations analysed applying the proposed design optimization method, are shown in Table 5. In particular, for each configuration the well diameter (D_w), the number of well lines (n_c), and the number of wells (n_w) are listed with the corresponding volume of adsorbing material (V_{Ad}) obtained and related costs. The height of all PAB-D wells (H) was kept constant and equal to the aquifer thickness (H=8 m).

As reported, the PAB-D Configurations #1-3 and #4-6 require two passive well lines (n_c=2) and one passive well line (n_c=1), respectively. It is possible to observe that, in all configurations, the number of wells (n_w) decreases by increasing D_w. In particular, by reducing n_c from two lines to one, a significant reduction of about 50% of n_w is obtained. Furthermore, at a constant number of well lines, V_{Ad} increases with D_w. However, passing from Configuration #3 to Configuration #4, a reduction of V_{Ad} was obtained, despite the increase of the well diameter, due to a reduction of the number of wells. The cost analysis as a function of well diameter (D_w) is depicted in Figure 3. As shown, C_{Ad} increases almost monotonically with D_w (which in turn influenced the number of well lines required), while C_{well} follows an opposite trend because of the smaller number of wells needed (Table 5), although their unit costs are more expensive (Table 4). In particular, C_{well} results higher than C_{Ad} for configurations with two passive well lines (Configurations #1-3), while the opposite ranking can be observed for configurations with a single well line (Configurations #4-6). Moreover, by increasing D_w, a higher incidence of C_{Ad} on C_R can be observed, which becomes 50% higher in the configurations with only one well line (Configurations #4-6). Since the monitoring cost (C_M) was considered equal to 250,000€ for all configurations, the minimum of C_R occurs when the increase of C_{Ad} and the decrease of C_{well} compensates.

The lowest remediation cost C_R was obtained for Configuration #4, i.e. with a well diameter equal to 0.8m, which also had the highest reduction in C_{Ad} (Figure 3).

Table 5. Results of the methodological approach to PAB-D optimisation

Figure 3. Cost trends as a function of well diameter

In Figure 4, for the optimised PAB-D configuration (i.e. Configuration #4 – D_w=0.8 m), the barrier inlet (C_{in}) and outlet (C_{out}) maximum benzene concentrations are represented over time as breakthrough curves. In particular, these curves were determined via COMSOL Multi-physics®, by positioning two observation points at both ends of the most external PAB-D well lines (representing the PAB-D inlet and outlet) along the groundwater flow direction, where the highest benzene concentrations were detected. As shown, an operating time of about 20 years is required to capture the whole polluted plume and to remediate the aquifer. Moreover, in order to verify the absence of benzene desorption from the barrier at concentrations higher than the Italian regulatory limit (C_{lim}=1 μg L^{-1}), the PAB-D efficiency was tested for an operating time of 100 years. As sketched, for the whole time simulated, the outlet benzene concentration is always lower than 1 μg L^{-1}.

Finally, a comparison between a Continuous PAB (PAB-C) (Santonastaso et al. 2015), designed for the remediation of the same study area, and the optimised PAB-D was carried out. The values of the geometrical parameters of both PAB-C and PAB-D, including the corresponding total adsorbing material volume and remediation costs, are reported in Table 6. The comparison shows that a 40% reduction of the adsorbing material volume (ΔV_{ad}) and a 28% reduction of the remediation costs (ΔC_R) can be achieved by using the optimised PAB-D (Configuration #4).

Figure 4. Breakthrough curves for the optimised PAB-D

Table 6. Comparison between PAB-C and the optimised PAB-D

5. CONCLUSIONS

This paper presents a methodological approach for PAB-D optimisation. The method is based on the definition of a set of PAB-D configurations, all of them allowing the capture of the contaminated plume and the remediation of the aquifer considered, and on the individuation of the most cost-efficient optimized configuration by comparing their respective costs. The PAB-D configurations were identified by varying their well diameter (D_w) and by assuming that both the distance between two consecutive passive wells (I) and the line-to-line distance (d_c) depend on D_w. The design optimization technique was aimed at minimising the adsorbing material volume of the PAB-D configurations and to identify the PAB-D configuration with the lowest remediation cost. This was calculated as the sum of well drilling costs, adsorbing material costs and monitoring costs.

Results show that a lower volume of adsorbing material can be obtained by increasing the number of the PAB-D wells and the configuration with D_w=0.8 m, I=1.6 m and d_c=0.8 m resulted to be the best optimised PAB-D layout, since the remediation cost was the lowest among those of the configurations tested. Moreover, the absence of benzene desorption phenomena from the barrier at concentrations higher than the Italian regulatory limit was verified, since for the whole operating time simulated, the PAB-D outlet benzene concentration was everywhere lower than 1 $\mu g\ L^{-1}$.

Finally, a comparison with a Continuous PAB, applied for the remediation of the same site, shows that by adopting the optimised PAB-D configuration, the adsorbing material volume and the remediation costs are reduced by 28% and 40%, respectively.

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Table 1 Main characteristics of the study area

Aquifer characteristic	
Total extent, A [ha]	225
Aquifer average piezometric level, H_w [m]	8
Piezometric gradient, J [m m^{-1}]	0.01
Porosity, n_s [-]	0.25
Dry soil bulk density, ρ_s [kg m^{-3}]	1,400
Hydraulic conductivity, K_s [m s^{-1}]	5×10^{-5}
Longitudinal dispersivity, α_x [m]	1
Transverse dispersivity, α_y [m]	0.1
Benzene molecular diffusion coefficient, D_{iff} [m^2 s^{-1}]	10^{-8}

Table 2 Main characteristics of the adsorbing material

Adsorbing material characteristics	
Porosity, n_b [-]	0.45
ACs bulk density, ρ_b [kg m^{-3}]	520
Hydraulic conductivity, K_{PAB} [m s^{-1}]	10^{-3}
Longitudinal dispersivity, α_{xPAB} [m]	0.05
Transverse dispersivity, α_{yPAB} [m]	0.005
AC BET surface area, S_{bet} [m^2 g^{-1}]	1.116
AC average pore diameter, d_{pore} [nm]	233.5

Table 3 Set of configurations considered for the design optimization

PAB-D Configuration #	D_w **[m]**	$I = 2{*}D_w$ **[m]**	$d_c = D_w$ **[m]**
1	0.4	0.8	0.4
2	0.5	1.0	0.5
3	0.6	1.2	0.6
4	0.8	1.6	0.8
5	1.0	2.0	1.0
6	1.2	2.4	1.2

Table 4 PAB-D unit costs

C_{well}		C_{Ad}	C_M
***D_w* [m]**	**Unit cost [€ m^{-1}]**	**Unit cost [€/m^3_{Ad}]**	**[€]**
0.4	47	780	250,000
0.5	51		
0.6	57		
0.8	69		
1.0	87		
1.2	103		

Table 5 Results of the methodological approach to PAB-D optimisation

PAB-D Configuration #	D_w [m]	H [m]	n_c	n_w	V_{Ad} [m^3]	C_{well} [€]	C_{Ad} [€]	C_R [€]	Incidence of C_{Ad} on C_R [%]
1	0.4	8	2	788	1009	1,626,432	786,739	2,663,171	30
2	0.5	8	2	610	1220	1,376,160	951,600	2,577,760	37
3	0.6	8	2	540	1555	1,321,920	1,213,056	2,784,976	44
4	0.8	8	1	257	1316	703,152	1,026,355	1,979,507	52
5	1.0	8	1	205	1640	678,960	1,279,200	2,208,160	58
6	1.2	8	1	158	1820	659,808	1,419,725	2,329,533	61

Table 6 Comparison between PAB-C and the optimised PAB-D

	Height [m]	Width [m]	Length [m]	V_{ad} [m^3]	ΔV_{ad} [%]	C_R [€]	ΔC_R [%]
PAB-C	8	0.57	400	1,824		3,304,720	
optimised PAB-D	8	0.8	257 x 0.8	1,316	28	1,979,507	40

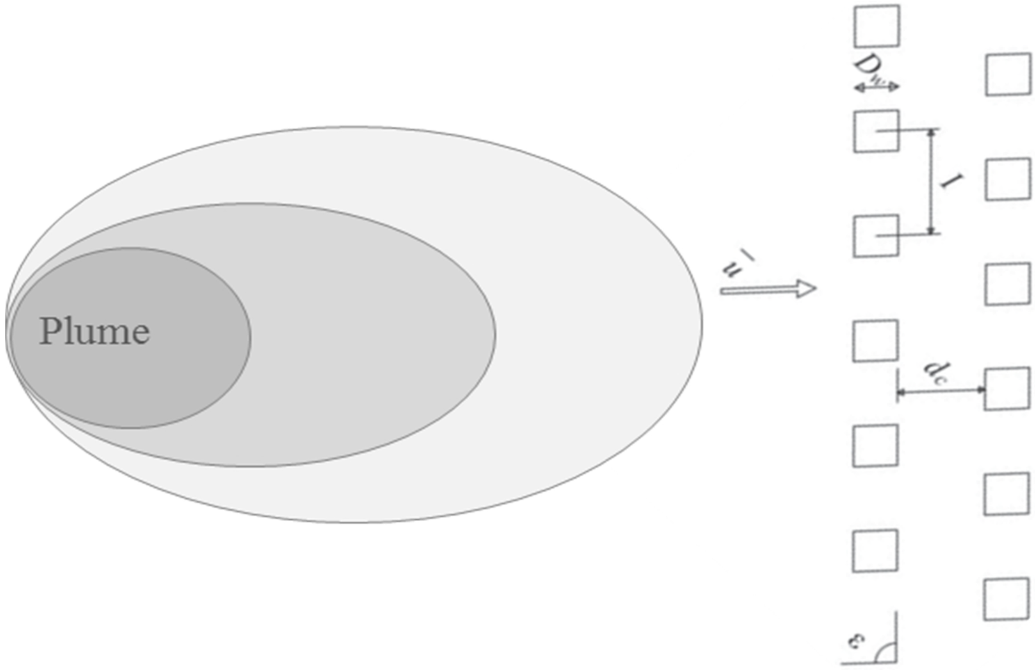

Fig. 1 Design parameters of a PAB-D (Bortone et al. 2013)

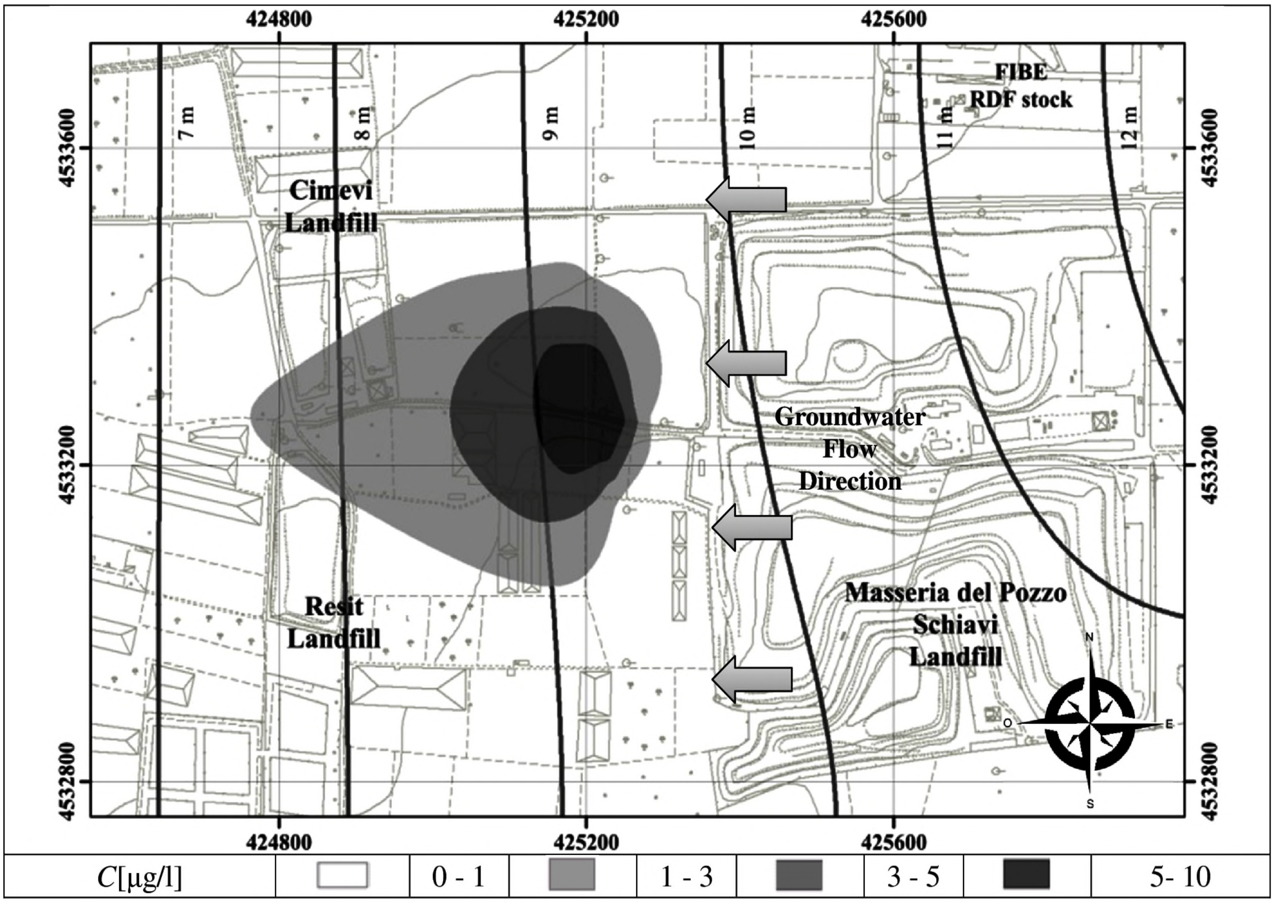

Fig. 2 Benzene iso-concentrations and groundwater piezometry of the study area

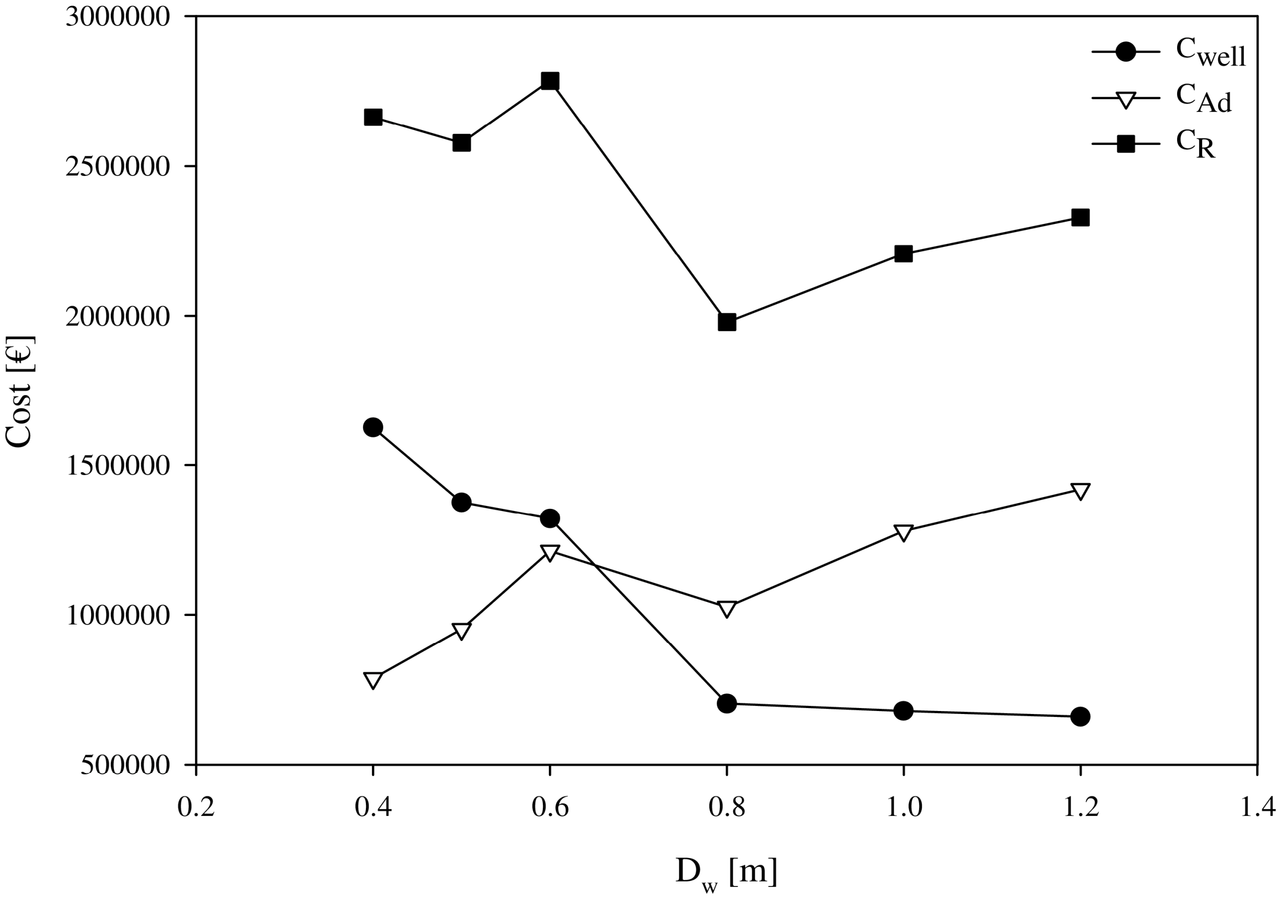

Fig. 3 Cost trends as a function of well diameter

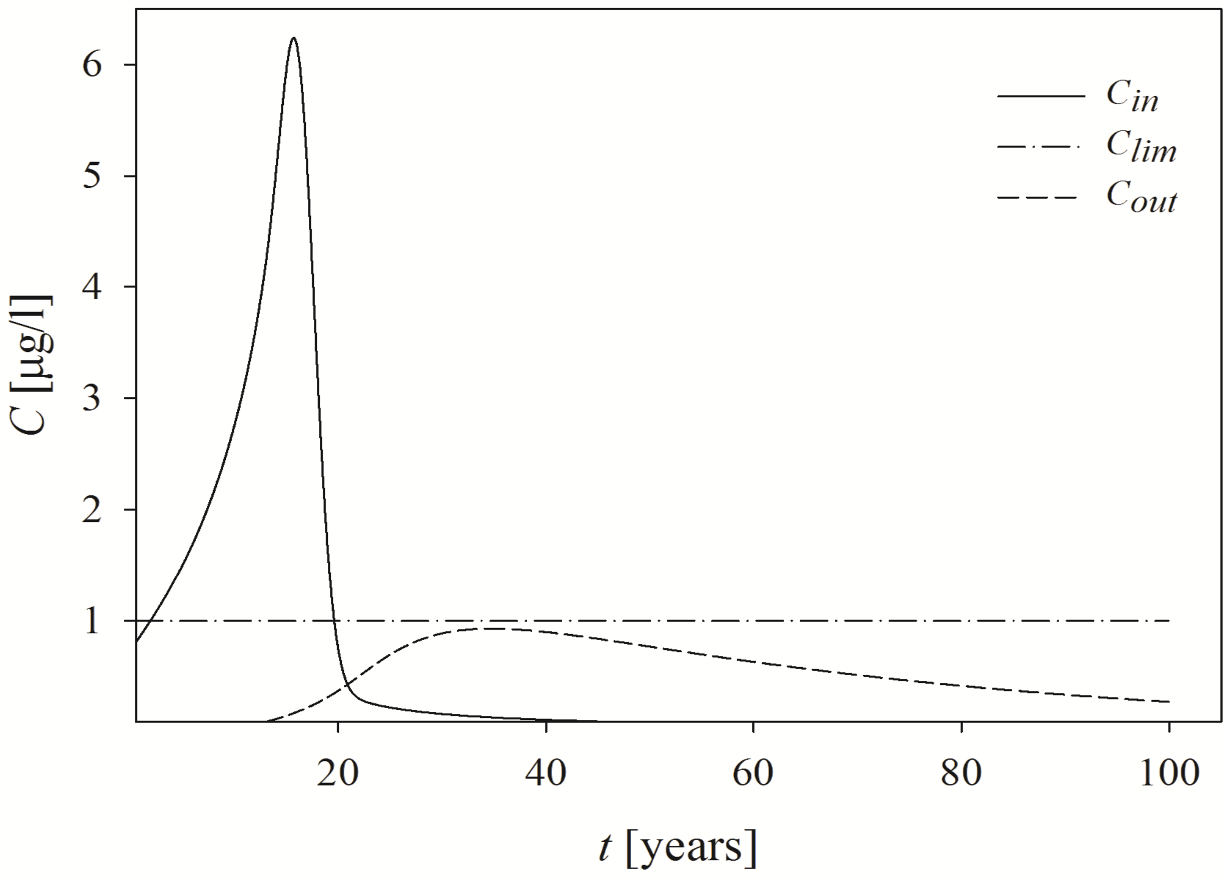

Fig. 4 Breakthrough curves for the optimised PAB-D

Discontinuous permeable adsorptive barrier design and cost analysis: a methodological approach to optimisation

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2017-09-19

Santonastaso, G.F., Bortone, I., Chianese, S. et al. Discontinuous permeable adsorptive barrier design and cost analysis: a methodological approach to optimisation. Environmental Science and Pollution Research, September 2018, Volume 25, Issue 27, pp 26793–26800

https://doi.org/10.1007/s11356-017-0220-y