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Two-objective Optimization for Optimal Design of the Multi-layered Permeable Reactive Barriers

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Abstract. The design, construction and management of engineering projects tend to be large scale, indivisible, and long-term facilities, with investments taking place in waves. This investment process due to constant further development has become a critical issue in the world management of civil engineering with regard to sectors of the national and private economy. These kinds of investments cannot be limited to solving just the mechanical problem. They should be designed with consideration of their life cycle, all costs of the project and construction stage, as well as what will be obtained during the lifetime of the investment. Due to the increasing environmental contamination, especially soil and ground-water, the need of restoration of these degraded lands for construction investment has emerged. Nowadays, the remediation technologies are more often focused on using passive engineering constructions installed in the ground, for example permeable reactive barriers (PRB) which allow for land use during decontamination processes. As with any investment, information about the costs of remediation technologies is as significant in determining their final commercial success as are efficiencies in the data. Technology investors need to have consistent cost information to conclude whether the technology will be economical or not. In the case of PRB technologies, the installation is a major investment cost, where one of the biggest drivers are material costs. The most important parameters for PRB cost and design are dimensions (thickness, length and height should be enough to treat the entire width of contaminants and to prevent their migration). The most important challenge is to determine the optimal thickness of a PRB, which provides the residence time appropriate for reducing the concentration of contaminants. In an engineering investment which involves designing, systems and decision making, optimization is crucial in creating best design subjects irrespective of constraints. In this paper two-objective optimization methods for multi-layered PRB design are considered. The proposed methods are characterized by following special features: elimination of a time-consuming simulation model; application of a universal, simple Excel spreadsheet-based optimisation model that calculates minimum cost of PRB using solver; and the usage of real input variability based on literature and laboratory tests. In view of minimizing cost of reactive materials and maximizing the resident time of contamination, the required thicknesses of PRB layers: activated carbon, zeolite and zero valent iron were calculated.

1. Introduction

Nowadays, around the world an increasing investment in civil engineering project is observed. The large engineering and construction projects (LECPs) have become symbols of economic prosperity in many countries of Asia, Africa, South America and West Europe. The main role of these project realizations is to serve the extensive economic interest of the country and maximize the prosperity of all society. The realization of civil works as well as construction of large buildings and infrastructure may directly achieve an increase in the economic growth through the creation of thousands of new jobs, businesses and income from tourism [1]. On the other hand, we see the super multinational construction and infrastructure projects, which are no longer inhibited by borders. These projects bring interconnectedness, complexity and new major trends, which are the rise of the mega general contractors (the leading and main domestic firms have become subcontractors to global, cross-border firms) and digitalization of the whole investment process (e.g. plan, design, construct, logistic and transport, management). In the developing countries, these trends create the need for raising urbanization and global construction. In developed countries, engineering projects are focused on more modern, sustainable, environmental friendly and “smart” [2].

In general, design, construction and management of engineering project have become large scale, indivisible and long-term facilities, with investments taking place in waves. One of the most important aspects to be considered is a complete construction project. During the design process of engineering constructions one of the main issues is the mechanical analysis with regards to the strength and strain parameters of the subsoil. The evaluation of mechanical properties of the subsoil is of vital importance when these soils constitute a foundation for earthen structures or are used as material for their realization. Moreover, the main consideration in any building design are loads, which describe the nature and scale of hazards or external forces that the construction must sustain to provide a reasonable performance for its entire lifetime. The predicted loads are depended on a building’s projected use (occupancy and function), configuration (shape and size), and localization (climate and site conditions). Finally, the type and scale of design loads affect decisions concerning the selection of material, construction details, and architectural configuration [3]. Over the past years the application of mechanics in engineering practice has undergone significant changes as a result of developments in computer technology. In addition, based on computing capability enhancement, higher speed, and increasing information storage, the software solutions have become capable of analysing problems of ever-increasing complexity and reliability [4]. However, these kinds of investments cannot be limited to solving just the mechanical problem during planning and design stage. They should be designed taking into account their life cycle and all costs incurred during the entire investment process, including project and construction costs, as well as the operation of a given engineering project [5, 6].

More and more often in the construction market obtaining the lands for development becomes very difficult due to big competition and contamination. The need for the restoration of degraded lands in the urban site is constantly growing. Post-industrial areas are attractive for their location near city centres or for their vicinity to the central parts of cities. The regeneration of brownfields seems to be a solution for urban economy and development of the cities. The general problem with these sites is associated with significant contamination of subsoil and groundwater by a mixture of many substances [7]. Nowadays, the remediation technologies are more often focused on using passive engineering constructions installed in the ground, for example permeable reactive barriers (PRB) which allows for land use during decontamination processes. As with any investment, information about the costs of remediation technologies is as significant in determining their final commercial success as are efficient data. Technology investors need to have consistent cost information to conclude whether the technology will prove economical [8]. Good practice in environmental cleansing projects is the analysis of archival unit costs, which may indicate the amount of pollutants processed and the volatility of historical data, as well as enable the comparison of options and selection of appropriate remedies [9]. During the past several years, the most frequently applied methods to clean-up contaminated media financed by public budget were the following: thermal desorption, soil vapour extraction (SVE), on-site incineration, groundwater pump-and-treat systems, bioremediation, and permeable reactive barriers (PRBs) [9]. The first four methods are examples of active remediation technologies of generally high energy consumption, which could lead to new environmental problems. Therefore, nowadays on remediation market the trend of using more efficient and economically passive techniques like bioremediation and PRBs are observed [10]. Additionally, the PRBs technology allows for commercial and developer use of the land during soil and groundwater clean-up process.

In this paper, a practical model for PBR design optimization is developed using the two-objective model. In the case of PRB technologies, the installation is a major investment costs, where one of the biggest drivers are material costs. The most important parameters for PRB cost and design are dimensions. The determination of the optimal thickness of a PRB, which provides a residence time appropriate for reducing the concentration of contaminants, represented a major challenge. The proposed method is characterized by following special features: elimination of a time-consuming simulation model; application of a universal, simple Excel spreadsheet-based optimization model that calculates minimum cost of PRB using solver; and the usage of real input variability based on literature and laboratory tests. In view of cost minimization of the reactive materials and maximization of the resident time of contamination, the required thicknesses of PRB layers; modified construction aggregate, activated carbon, and zero valent iron were calculated.

2. Optimization of remediation projects

During the last decades, the increasing investment in remediation project has been observed. The significant attention is paid to minimizing capital, operating, and maintenance costs and maximizing contaminant removal effectiveness. Furthermore, technical restrictions and regulatory remediation standards must be observed [11, 12].

Optimization of groundwater remediation activities could be performed by compilation of design problems in mathematical format acceptable to the optimization algorithm. In general, there is no universal method of defining every engineering design problem. Usually, the optimization procedure is applied to maximize the efficiency of process or to minimize the cost. In order to achieve the optimal or an approved solution, the optimization algorithm is performed iteratively. Termination of the whole procedure in many engineering cases is reached indirectly by comparing a set of chosen design solutions and approving the best one. To avoid mistakes, the optimization starts with one or more design solutions, which are then iteratively verified in order to achieve the true optimum solution. In most cases, the optimization procedure began from single-variable function, which could be used in multivariable optimization algorithms as unidirectional search methods. Further calculations are continued by applying algorithms to solve the problems contained in multiple design variables with unconstrained objective functions [13].

In most cases, the optimization made the entire procedure cost-effective and widely implemented. Thus, engineering problems are solved by using straight or estimated mathematical search methods e.g. linear programming, integer programming, dynamic programming or branch-and-bound techniques to arrive at the optimum solution for moderate-size problems [14]. With the development of computing capabilities of computers, several algorithms were implemented to describe groundwater and contaminated transport for the determination of an optimal remediation strategy [15]. The several optimization procedures were obtained in order to minimize cost and time of pump and treat and surfactant-enhanced flushing remediation technologies. Minsker and Shoemaker [16] developed the nonlinear optimization algorithm to increase monitoring of in-situ bioremediation process. Thus, Huang et al. [17] applied an integrated simulation-optimization model for modelling and control remediation process at DNAPL-contaminated sites, so did Schaerlaekens [18] and Quang [19], who used multi-objective optimization for this purpose. However, there are only several reports of the procedure to optimize the design of PRB. Guerin [20], Higgins and Olson [21] applied simulation-based empirical methods. Furthermore, nonlinear optimization calculations of dimensional parameters of PRBs were performed by Painter [22] and Craig [23]. On the other hand, Nardo [15] developed a simulation – based heuristic procedure to optimize the position and dimensions of barrier built with activated carbon. The design and optimization of effective work of PRB count the hydrological and geotechnical properties of entire contaminated site. Thus to support this work several simultaneous numerical modelling programs (FEFLOW 5.3 by WASY GmbH, ChemFlux by SoilVision, Visual ModFlow by Waterloo Hydrogeologic) are used. They could be used for ground water flow and contaminant transport, however not for PBR design optimization. The situation becomes more complicated in case of MPRB design. This software is highly suitable for preliminary barrier sizing, but an optimal procedure is required to specified dimensions. Furthermore, the computer modelling is a time-consuming process that requires additional software. Moreover, optimizing the design of PRB in the field scale is much more challenging because of the enormous and intricate solution space [14]. In some cases of remediation process of optimization there is the need for finding a global optimal solution in a multi-optimal problem, where the problem contains a number of local and global optimal solutions and the objective is to find the global optimal solution [13]. For this reasons, the two – objective optimization model in common and easily accessible software could be helpful in PRB design.

3. The thickness optimization of multi-layered PRB

A PRB design is a very demanding and complex task including hydraulic, geological and contaminant characterisation. The most important parameters for PRB cost and design are dimensions (thickness, length and height should be enough to treat the entire width of contaminates and to prevent their migration). The greatest challenge is to determine the optimal thickness of a PRB, which provides a residence time appropriate for reducing the concentration of contaminants and effective work of the barrier. In engineering investment which involves designing, systems and decision making, optimization is crucial in creation of best design subjects despite the constraints. The design of PRB for contaminated groundwater as well as single objective optimization model for the design of multi-layered PRB (MPBR) was performed in work of Polonski et al. [24]. In previous studies, there were two variants of the objective function - the maximization of residence time and minimization of total costs. The optimum solution was identified on the basis of a comparison of resolved functions in longevity and cost. However, the true optimization solution of PRB's thickness should be conducted with simultaneous consideration of two divergent criteria.

In order to achieve this goal, it was assumed that the final answer to the question of optimization will be kept as a solution of two partial functions. In the optimization task the minimization of maximum absolute deviation of time and costs Z from their optimal values were performed according to the formula [25]:

$$Min\,Z: \quad Z = max\{w_T \cdot K_T + \rho \cdot (K_T + K_C);\ w_C \cdot K_C + \rho \cdot (K_T + K_C)\} \tag{1}$$

where: w_T – weight time criterion; w_C – weight cost criterion; K_T – normalized value of time partial function of the objective, K_C – normalized value of cost partial function of the objective, ρ - correction factor.

The correction factor could be obtained as follows:

$$\rho = \frac{1}{d} \cdot max(w_T \cdot K_T; w_C \cdot K_C) \tag{2}$$

where: d – a sufficiently large number.

The part of main equation with ρ allows to reduce weakly-not-dominated solutions, which means that the second part searches for the solutions that generate first and chooses the best ones.

In calculations the criterion Z was normalized using zero unitization method based on the span of the minimum and maximum values. The minimum and maximum values of criteria (time and cost) were obtained by solving a single-variable function and looking up the maximum and minimum values in a range based on specific restrictions. Due to the fact that partial criteria did not pursue the same extreme, an additional criterion was distinguished as a destimulant and stimulant. The working time of MPRB strived to maximum and was an destimulant, whereas the total cost of MPRB was a stimulant strived to minimum. The normalized two - objective function of partial criteria can be examined using the following formulas:

$$\text{normalized destimulant: } K_T = \frac{Z_{Tmax} - Z_T}{Z_{Tmax} - Z_{Tmin}} \tag{3}$$

$$\text{normalized stimulant : } K_C = \frac{Z_C - Z_{Cmin}}{Z_{Cmax} - Z_{Cmin}} \tag{4}$$

where: Z_{Tmax}, Z_{Tmin} – maximum and minimum time partial function of the objective (one – criterion criterion) with existing restrictions; Z_{Cmax}, Z_{Cmin} – maximum and minimum cost partial function of the objective (one – criterion) with existing restrictions; Z_T –partial function of the objective for time, Z_C – partial function of the objective for cost.

As in previous studies [24] the optimization calculations were performed in Microsoft Office Excel add-in program SOLVER with the difference of using the "GRG" nonlinear algorithm opposite to linear “LP Simplex”. In order to increase the efficiency of optimization procedure the macro VBA was written, which automated the process of calculating the efficiency of each unit weight variations (i.e. lower boundary, higher boundary and literation - pitch). The calculation procedure was carried out in a loop differentiating the single results from the single-variable analysis (cost or time) by changing the weight. The sum of all criteria weights was equal to 1 ($w_T + w_C = 1$). Moreover, the influence of weight to the final results was analysed. The whole procedure for optimization of the design of MPRB consisted of two stages: 1) calculation of normalized partial functions with imposed restrictions where the criteria were time run to max. and cost run for min. criteria, and 2) resolved iteratively the global function Z to achieve the optimal solutions. Furthermore, the two staged procedure was included in developed macro VBA.

In this case the study led to assume that groundwater is contaminated by a mixture of heavy metals (Cd, Cu, Ni, Pb, Zn). Based on performed laboratory test results [24, 26] the remediation of polluted site using MPRB with different layers of silica spongolite (SS), zeolite (ZE) and activated carbon (GAC) was proposed. During the contact of flowing contaminated water with reactive materials the following clean-up process could be observed: reduction and/or precipitation, ion-exchange and sorption [26-30]. In order to be cost effective, the MPRB has to be characterised with minimum dimensions.

In the optimization model the unknown values were thicknesses of single layers (b_m) in the MPRB. Accordingly, for the optimization calculations, the following general restrictions were taken into account:

- number of used materials (M) equal to 3;
- barrier height (h) and length (L) each equal to 1 m,
- minimum thickness of one layer - 0.1 m;
- maximum width of the entire barrier - 2 m;
- minimum thickness of entire barrier varied from 1.5 m to 1.9 m;
- minimum retardation time of SS layer - 100 days.

If necessary, the above restrictions can be modified with taking into account the specified field condition and using materials for barrier construction.

Inputs to the optimization model were based on the cost of buying 1 Mg of reactive material and the parameters determined from laboratory tests performed in the Department of Geotechnical Engineering of the Warsaw University of Life Sciences [27, 31] and were as follows: flow velocity v_m [m/s], retardation factor R_m for mixtures of heavy metals [-], and density ρ_m [kg/m^3]. The values of the input parameters are presented in Table 1.

Table 1. Model input parameters

M	**Reactive material**	v_m **[m/s]**	ρ_m **[kg/m3]**	R_m **[-]**	$cost_m$ **[euro]**
1	SS	0.00000476	1.21	228.20	17.28
2	ZE	0.00000213	1.05	882.37	32.50
3	GAC	0.0000016	0.45	33.49	1070.43

The required resident time for contamination removal can be calculated using this equation [36]:

$$t_{Rm} = \frac{b_m R_m}{v_m} \tag{5}$$

where: b_m – thickness of a single layer of WPBR [m], R_m – retardation factor of a single layer [–], v_m – flow velocity through a single layer m [m/s]. The cost of a single layer of a MPRB $cost_m$ (h & L = 1 m) can be calculated using the following formula:

$$cost_m = b_m \cdot \rho_m \cdot cost_m \tag{6}$$

The total purchase cost of reactive materials (*cost*) filling a WPBR is the sum of the costs of single layers and it is as follows:

$$cost = \sum_{m=1}^{M} b_m \cdot \rho_m \cdot cost_m \tag{7}$$

4. Results and discussions

In Table 2, the main results of two - objective optimization were reported. The calculations were performed for two different ranges of minimum and maximum thickness of MPRB. During the first optimization procedure, the minimum thickness b was equal to 1.5, whereas for the second series this dimension was 1.7 m and at the definitive third series was 1.9 m. The range reduction of searched thickness values of MPRB has an impact on the overall performance of the functions Z and calculated thickness. The results showed that in case of these three series the layers of thickness were changed only for SS and ZE. This was the effect of the materials' parameters, especially due to the value of retardation factor R_m. The greatest value of this parameter was noted for GAC, for the reason of its large internal surface area, which is known for its high affinity to removal heavy metals by adsorption process. Therefore, regardless of the imposed limitation of the barrier thickness, the thickness of this layer would be constantly the least (also because of its costs), however still sufficient for effective clean-up processes. The user of this optimization model e.g. designer from all results obtained for different range of thickness and weight w from 0 to 0.2, can choose the optimal MPRB system according to the needs and prevailing conditions. After the series of optimization calculation the obtained results of layers' thickness indicated that analysed MPRB should have the following values of b_m: GAC – 0.1 m, ZE – 1.6 m, and SS - 0.2 m.

Table 2. Calculated results

Weight						**Layers thickness b_m [m]**			**MPRB thickness**
w_T	Z_T [days]	Z_C [euro]	K_T [days]	K_C [euro]	Z	SS	ZE	GAC	b [m]
				***b* 1.9 – 2.0**					
0.2	7961.3	163.38	0.011	0.011	0.011	0.180	1.635	0.100	1.915
0.18	7911.3	163.04	0.011	0.011	0.011	0.180	1.624	0.100	1.904
0.16	7848.0	162.75	0.011	0.011	0.011	0.190	1.610	0.100	1.900
0.14	7767.0	162.46	0.011	0.011	0.011	0.209	1.591	0.100	1.900
0.12	7662.1	162.08	0.011	0.011	0.011	0.234	1.566	0.100	1.900
0.1	7520.9	161.57	0.011	0.011	0.011	0.267	1.533	0.100	1.900
0.08	7320.8	160.86	0.011	0.011	0.011	0.315	1.485	0.100	1.900
0.06	7015.0	159.76	0.011	0.011	0.011	0.387	1.413	0.100	1.900
0.04	6490.1	157.88	0.010	0.010	0.010	0.511	1.289	0.100	1.900
0.02	5193.9	154.75	0.009	0.009	0.009	0.929	0.971	0.100	2.000
0	1447.0	139.78	0.000	0.000	0.000	1.700	0.100	0.100	1.900
				***b* 1.7 – 2.0**					
0.2	7905.9	163.00	0.012	0.012	0.012	0.180	1.623	0.100	1.903
0.18	7849.1	162.62	0.013	0.013	0.013	0.180	1.611	0.100	1.891
0.16	7780.3	162.15	0.013	0.013	0.013	0.180	1.597	0.100	1.877
0.14	7695.4	161.58	0.013	0.013	0.013	0.180	1.579	0.100	1.859
0.12	7587.9	160.85	0.013	0.013	0.013	0.180	1.557	0.100	1.837
0.1	7447.4	159.90	0.012	0.012	0.012	0.180	1.527	0.100	1.808
0.08	7256.0	158.60	0.012	0.012	0.012	0.180	1.487	0.100	1.768
0.06	6979.9	156.73	0.011	0.011	0.011	0.180	1.430	0.100	1.710
0.04	6105.3	158.02	0.012	0.012	0.012	0.714	1.186	0.100	2.000
0.02	4768.3	153.23	0.010	0.010	0.010	1.030	0.870	0.100	2.000
0	1336.0	136.32	0.000	0.000	0.000	1.500	0.100	0.100	1.700
				***b* 1.5 – 2.0**					
0.2	7850.0	162.63	0.014	0.014	0.014	0.180	1.611	0.100	1.892
0.18	7786.4	162.20	0.014	0.014	0.014	0.180	1.598	0.100	1.878
0.16	7709.4	161.67	0.014	0.014	0.014	0.180	1.582	0.100	1.862
0.14	7614.4	161.03	0.014	0.014	0.014	0.180	1.562	0.100	1.842
0.12	7494.0	160.21	0.014	0.014	0.014	0.180	1.537	0.100	1.817
0.1	7336.8	159.15	0.014	0.014	0.014	0.180	1.504	0.100	1.785
0.08	7122.8	157.70	0.013	0.013	0.013	0.180	1.460	0.100	1.740
0.06	6814.0	155.60	0.012	0.012	0.012	0.180	1.395	0.100	1.675
0.04	5834.6	157.05	0.014	0.014	0.014	0.778	1.122	0.100	2.000
0.02	4340.7	151.69	0.011	0.011	0.011	1.131	0.769	0.100	2.000
0	1225.0	132.86	0.000	0.000	0.000	1.300	0.100	0.100	1.500

All results of function *ZT* and *ZC* were presented in the graph. Figure 1 showed that in relation to the costs, time is characterized by relatively rapid growth. In series with the b min started from 1.5 and 1.7m the spread of results was observed. Better correlation between *ZT* and *ZC* was reported for series with the narrow scope of parameter *b*. Thus, the search for optimal solution should be performed in the place where the curve rises upwards and for series of narrow range of input restrictions.

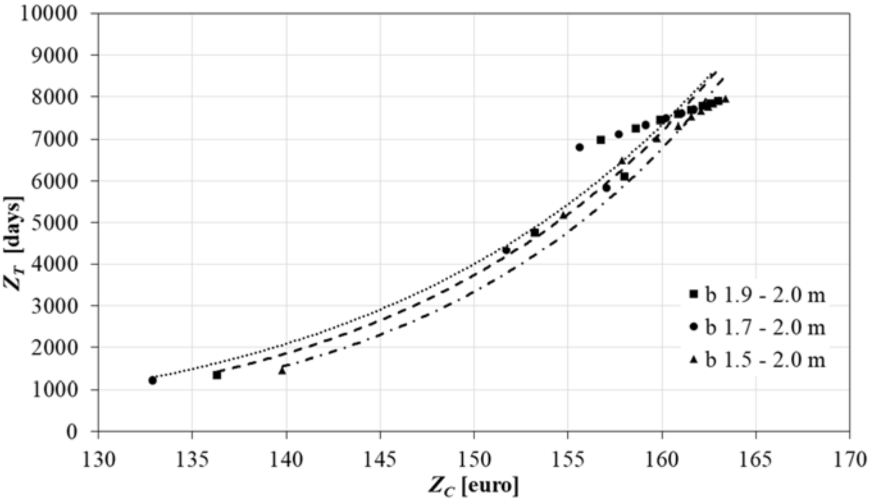

Figure 1. The relationship between total resident time for contamination removal and total costs of materials filling the MPRB

5. Conclusions

In today's world, the realization of large scale engineering projects is truly a global venture, driven by enhanced urbanization and development. Due to the lack of opportunities to find attractive lands for investment, remediation of contaminated brownfields localized near city centres or in the vicinity of central parts of the cities has become a great solution. The remediation technologies are more often focused on using passive engineering constructions e.g. permeable reactive barriers (PRB) that allowed for land use during clean - up processes. As with any investment, information about the costs and effective time of working PRB is necessary to plan and execute full remediation investment. The optimization for optimal design of the multi-layered PRB systems could be very helpful in this matter. In comparison to previous studies it is more appropriate to use multi – criteria optimization algorithm instead of one-criterion. By writing macro VBA the efficiency of optimization procedure was increased and automated. This improvement significantly reduced the calculation time and afforded for fast analysis of many calculation variants. The user of optimization model can choose the optimal MPRB system according to the needs and prevailing conditions. Furthermore, optimal solution should be performed in place where the curve of relationship between total time and cost rises upwards and for series of narrow range of input restrictions. The analysed MPBR after series of optimization under the admitted assumptions should have the following thickness of layers: GAC – 0.1 m, ZE – 1.6 m, and SS - 0.2 m. In summarizing, reported results showed that the dimension problem of PRB is non-linear. Consequently, the proposed two-objective non-linear optimization model is an effective and accessible tool to optimize the barrier dimension.

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