Performance Prediction of Permeable Reactive Barriers by Three-Dimensional Groundwater Flow Simulation

Young Wook Chung, Juyoul Kim and Sung-Ho Kong

***Abstract*—Various analytical methods for describing the hydraulic behavior of a permeable reactive barrier (PRB) are developed based on a three-dimensional approximation of the groundwater flow system. To simulate the actual geological groundwater system, modeling was proposed in this study. Using MODFLOW module of the GMS software, the groundwater head and contaminants (BTEX; Benzene, Toluene, Ethyl benzene, and Xylene) concentration distribution model was developed. Based on these data and models, the optimal location of PRB installation was selected and the performance of PRB and the future response of Hydrogeological system were predicted by the model.**

***Index Terms*—GMS, groundwater modeling, MODFLOW, permeable reactive barrier.**

I. INTRODUCTION

Recently, the contamination of wastewater and groundwater by organic compounds has been concerned since the Industrial Revolution. These contaminated aqueous streams should be treated for the requirements of human being that increase demand of quality water resource. Physical, biological, and chemical treatment processes can treat organic compounds, which caused environmental problems. The pump-and treat system is the most widely used and studied, but it has been revealed to have a number of technical and practical limitations. In particular, it is a very expensive process, requiring continuous energy inputs for years [1]. Permeable Reactive Barrier (PRB) is one of the most famous alternative processes among passive decontamination methods. Typically, PRB consists of a trench filled with reactive material placed in the path of a contaminant plume. As groundwater passes through the PRB, contaminants are removed by chemical and/or biological reactions and/or sorption to the PRB material. Regardless of the removal mechanism, PRB performance depends on the placement of the barrier to capture the targeted contaminant plume and the residence time within the PRB to accomplish the remediation. Thus, adequate designs are required to intensively understand the groundwater flow system affected by the PRB.

The PRB treatment for the remediation of petroleum -contaminated groundwater system has a typical limitation for its durability. Over times, the contaminants, chemical and biological reaction products, and other debris can be absorbed to PRB material and cause the blockage of the PRB. To solve this problem, strong oxidants were introduced alternatively to trigger advanced oxidation process (AOP) to reduce this blockage and extend the durability of the PRB.

AOP is the most famous process among chemical oxidation. These are commonly generating the most powerful oxidant, hydroxyl radical (·OH). Among these, classic Fenton reaction is well known reaction since 1864 [2]. Classical Fenton reaction generates strong, non-selective oxidants, hydroxyl radicals reacting with ferrous salts and hydrogen peroxide (H2O2). Classic Fenton reaction have some disadvantages; 1) to apply to in or ex-situ treatment, extremely low pH was required, and 2) ferrous ion oxidize to ferric ion too fast to reduce, additional ferrous ion have to inject sequentially. In these days, different type of Fenton-like reaction, called ‘heterogeneous Fenton catalyst’ has been developed. Many researchers have been reported the various heterogeneous Fenton catalyst such as Nafion, polyethylene film, alginate gel beads, Nafion/glass fiber, silica fabrics and layered clays [3-5].

Modeling of groundwater flow through a PRB is regularly performed using a numerical simulator such as MODFLOW [6]. To begin with the modeling, geological variables should be classified and characterized. Based on these characterizations, the conceptual design could be accomplished to select what software could be applied for the modeling of the geological groundwater system. The selected software should be able to provide the model which can simulate the flow of the groundwater flow and the transport of contaminant based upon the conceptual geological model of specific area to be concerned.

II. BACKGROUND

A. *Permeable Reactive Barrier*

The permeable reactive barrier was introduced in the mid-1990s [7] as a passive alternative to active pump-and-treat remedial strategies. Since that time, a variety of pilot tests, field tests, and commercial installations have been implemented [8]. An important part of the design process for these barrier systems is a sound characterization of the aquifer hydrogeology and determination of the plume

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boundaries [9]. From this information, the PRB may be designed to 1) effectively capture the plume and 2) achieve a sufficient residence time within the PRB for the applicable reaction processes to accomplish the desired reduction in contaminant concentrations.

B. Groundwater Modeling

The groundwater modeling is the management tool for making a decision to provide the information about the groundwater system concerned and the future response of the system to be effects of management decision. In other words, model could provide future distribution of contaminant concentrations, water levels, plume direction, etc

A model may be described as a simplified version of an actual ground-water system that approximately simulates the relevant excitation-response relations of the actual system. Since the actual systems are very complex, simplification is needed to make a modeling plan. The simplification is established by the assumptions which express the nature of the actual system and those features of its behavior that are relevant to the problem under investigation.

The first step in the modeling process is the construction of a conceptual model consisting of a set of assumptions that verbally describe the system's composition, the transport processes that take place in it, the mechanisms that govern them, and the relevant medium properties. The assumptions in a conceptual model should involve to such items as:

- the geometry of the boundaries;
- the kind of solid matrix;
- the mode of flow in the aquifer;
- the flow regime;
- the properties of the water;
- the relevant state variables;
- sources and sinks of water and of relevant contaminants, within the domain and on its boundaries;
- the initial conditions within the considered domain; and
- the boundary conditions.

Selecting the appropriate conceptual model for a given problem is one of the most important steps in the modeling process. Oversimplification may lead to a model that lacks the required information, while undersimplification may result in a costly model, or in the lack of data required for model calibration and parameter estimation, or both.

The next step in the modeling process is to express the (verbal) conceptual model in the form of a mathematical model. The mathematical model consists of the following items:

- a definition of the geometry;
- an equation that expresses the balance of the considered extensive quantity;
- flux equations;
- constitutive equations;
- an equation that expresses initial conditions; and
- an equation that defines boundary conditions.

All the equations must be expressed in terms of the dependent variables selected for the problem. The selection of the appropriate variables to be used in a particular case depends on the available data. The number of equations included in the model must be equal to the number of dependent variables.

Based on the conceptual and mathematical model, the selection of numerical model and code is the next step. To select appropriate code, the availability and modifiability of the code should be considered to obtain optimal solution.

Considering the uncertainty of model, the calibration and following sensitivity analysis could be performed to obtain the appropriate solution of predictive runs. Every model must be calibrated before it can be used as a tool for predicting the behavior of a considered system. During the calibration phase, the initial estimates of model coefficients may be modified. The sensitivity analysis may be postponed until a numerical model and a code for its solution have been selected. Figure 1 illustrates a simple diagram of a model application process. Each phase of the process may consist of various steps [10].

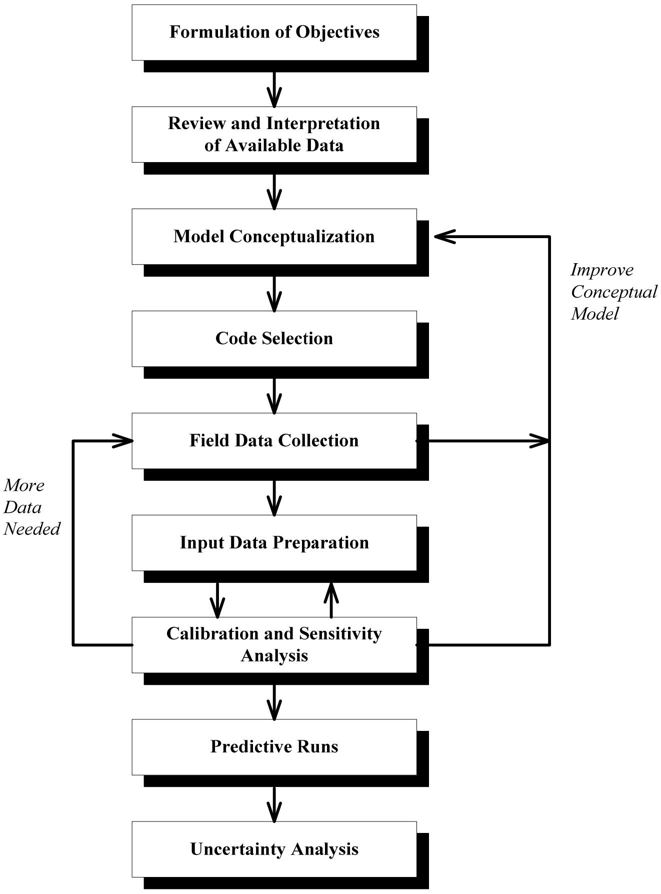

Figure 1. Goundwater Model Application Process.

III. SITE DESCRIPTION

The site around the quartermaster corps in which oil underground tanks were laid was selected to be investigated and researched. Figure 2 shows the 2-dimensional CAD drawing of this site. The underground oil tanks (circle marks) is located in northern area and railroads are laid from center to southeast. The proposed site in which the PRB would be installed is "C" area in the Figure 2, where a pump house is located. Each Mark of Figure 2 represents the location of monitoring well to measure the concentration of contaminants in pre-investigation. Based on the results of pre-investigation, the pump house is suspected of the contaminant source.

Figure 2. 2-Dimensional Drawing of Research Site

IV. MODELING RESULTS

According to the results of land survey on the site, full scope groundwater head model were accomplished as Figure 3. The groundwater head of the northwestern area where the oil tanks are located were higher than the south area. Because the direction of groundwater flow is generally perpendicular to the head distribution, the groundwater of this area would be supposed to flow from northwest to south.

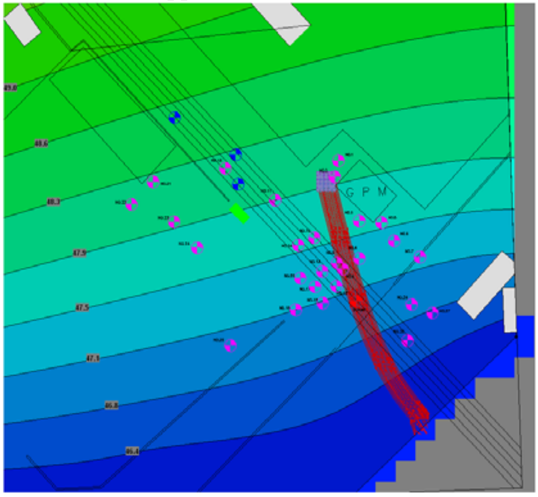

Figure 3. Groundwater Head Distribution Model and the presumed pathway of contaminants around GPM

Table 1 show the groundwater head data of each monitoring well located in the site. Table 2 is the hydraulic conductivity obtained from the conductivity test results of each monitoring well. Without the failed test results of MW-7 and MW-9, the applied hydraulic conductivity (0.00049) were determined from the geometric mean of the data from the other 8 monitoring well.

Figure 4 is enlargement of the groundwater head distribution of "C" area in the Figure 2. Each pink and blue mark represents monitoring well to measure the concentration of contaminants, hydraulic conductivity, and the head of water. Since the contaminant concentration of GPM area is relatively higher, this area is suspected to be the source. According to the groundwater head distribution model, the red line in the Figure 4 is presumed pathway of contaminants.

TABLE 1. GROUNDWATER HEAD OF EACH MONITORING WELL

Well No.	Groundwater Head(cm)
1	-
2	103
3	126
4	137
5	-
6	203
7	-
8	-
9	85
10	56
11	51
12	85
13	-
14	-
15	51
16	82
17	79
18	98
19	-
20	90
21	60
22	59
23	-
24	-
25	90
26	160
27	190

TABLE 2. HYDRAULIC CONDUCTIVITY DATA OF EACH MONITORING WELL

Well No.	K(cm/s)
MW-1	0.0001561
MW-2	0.0005572
MW-3	0.001209
MW-4	0.0001997
MW-5	0.001395
MW-6	0.000577
MW-7	failed
MW-8	0.0006745
MW-9	failed
MW-10	0.0002914

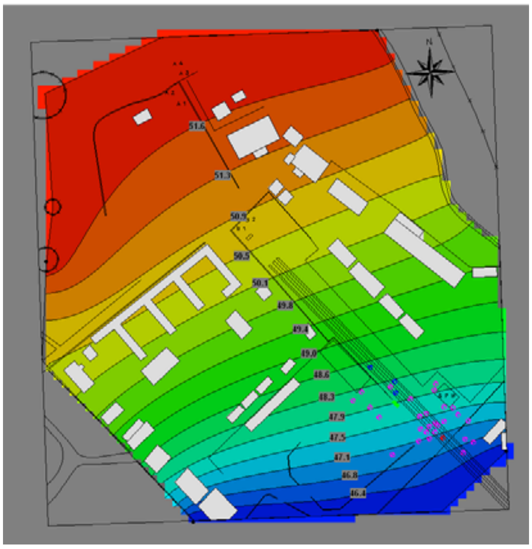

Figure 4. Groundwater Head Distribution Model of Research Site

V. PREDICTION OF HYDROGEOLOGICAL SYSTEM AND PRB PERFORMANCE

A. *Hydrogeological change*

For the understanding of the change of hydrogeological system after the installation of PRB, the groundwater head were measured via monitoring well of the site. Fig. 5 shows the change of groundwater head distribution due to installation of PRB.

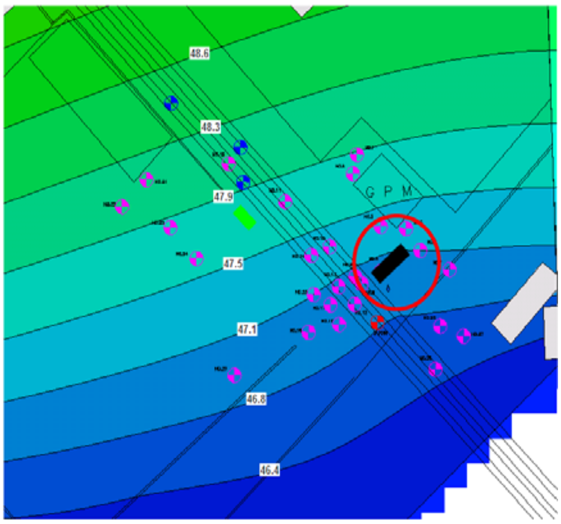

Figure 5. Groundwater Head Distribution Model after the Installation of PRB around GPM

Because of the installation of BRB, the groundwater head were a little lowered around GPM but the wide range of the hydrogeological system were hardly changed. In this manner, it is expectable that the pathway of contaminants presumed before the installation of PRB would not be changed.

B. *Performance Prediction of PRB*

Fig. 6 and 7 show the prediction of contaminant concentration distribution in 10 years before/after the installation of PRB. For the prediction, continuous leakage at the containment concentration of 6535 ppm was assumed. The PRB performance was predictable in comparing between Fig. 6 and 7.

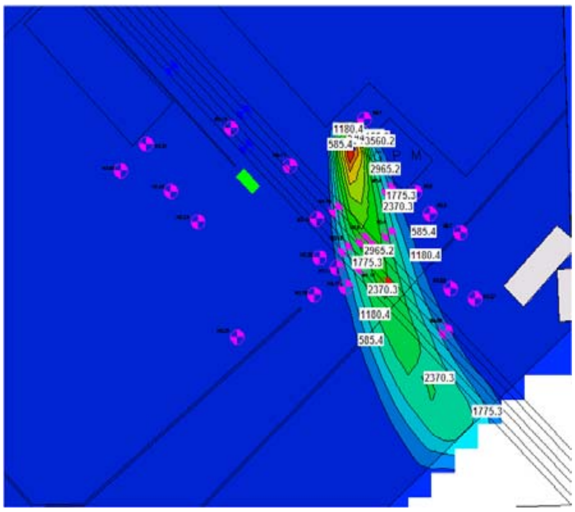

Figure 6. Concentration Distribution of Contaminant in 10 years – Before the Installation of PRB

Fig. 7 shows obviously that PRB is very effective for the prevention and of very soluble pollutant dispersion and very possible for the degradation to the expected level of pollution despite of its high volatility. Through the prediction of PRB performance, PRB is very applicable to the remedy of fuel contaminated groundwater and the possibility of the decrease of contaminant concentration was verified.

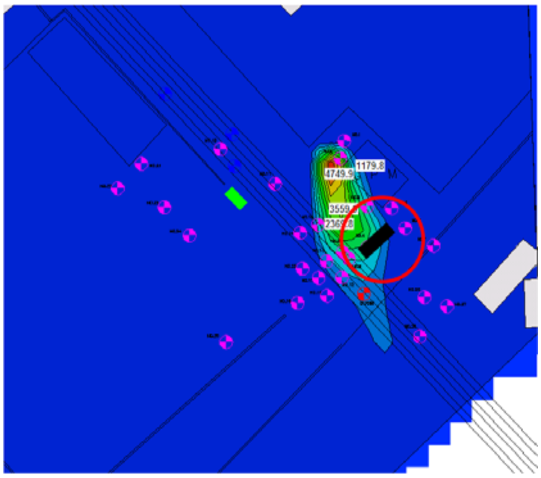

Figure 7. Concentration Distribution of Contaminant in 10 years – After the Installation of PRB

VI. CONCLUSION

For design and installation of PRB to remediate BTEX-contaminated area, the three dimensional groundwater flow simulation were introduced to find an optimal location, size, and direction of PRB. As figure 4 shows, PRB is proposed to be installed on the red line and perpendicularly direction to the red line. Through the comparison between the concentration distribution of contaminant predicted by the simulation before and after the PRB installation in 10 years, it was found that PRB is very applicable to the remedy of fuel contaminated groundwater.

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