2011 International Conference on Environment and BioScience
IPCBEE vol.21 (2011) © (2011) IACSIT Press, Singapore

Analysis of Passive Remediation of Contaminated Groundwater with Dimensionless Numbers

Jong Soo Cho[1 +], Soon Mi Kim[1] and Ioan Iordache[2]

[1] Catholic University of Korea, Kyunggi Do, Korea
[2] NRDICIT - ICIT Rm. Valcea, Romania

Abstract. On application of the passive remediation to the contaminated groundwater, the most important point is whether the target contaminant should decrease through reaction to the predetermined level within the selected distance. It is possible with dimensionless numbers such as Peclet number, *Pe*, 1st Damköhler number, Da_1, or 2nd Damköhler number, Da_2 to conduct the preliminary analysis. For the zero-valent iron permeable reactive barrier, it was possible to estimate the thickness of the reactive barrier wall to achieve the desired concentration of the effluent. In this paper, the analysis of real field data is presented with the analytical solutions of the convective-dispersive-1st order reaction rate equation.

Keywords: dimensionless numbers, advection-dispersion-reaction equation, permeable reactive barrier

1. Introduction

A permeable reactive barrier (PRB) is a control measure installed in the contaminated groundwater layer to passively degrade the contaminant. Along with the groundwater flow, the contaminant passes through the permeable reactive barrier and reacts with the packing materials such as zero-valent iron powder or biologically-induced reactive media. The contaminant becomes degraded or precipitated so that when it reaches the end of the reactive zone, its concentration becomes lower than the permissible limit. In the laboratory, the contaminant is characterized, the proper reactive material is searched, the system feasibility is tested and the design factors are obtained. In the actual field site, hydrogeological characteristics, contaminant distribution, and geochemical properties should be obtained to optimize the design of the system. If necessary, a pilot scale should be conducted. Since this is a passive remedial measure, it may require a long-term monitoring plan. After the system design, the reactive wall and monitoring wells are installed and the operation of the system is initiated with performance tests through sampling at the wells. The contaminant concentration after the reactive wall should satisfy the remedial goals. In this paper, the thickness of the reactive barrier is defined as the characteristic length, *L*. The schematic diagram of the PRB is in Figure 1.

2. Fate and Transport of Contaminant in Groundwater

Contaminant fate and transport in groundwater can be expressed with an one-dimensional advection-dispersion-reaction equation and boundary conditions. At the steady state, the equation becomes

$$0 = \mathrm{D}\frac{\mathrm{d}^2\mathrm{C}}{\mathrm{dx}^2} - V\frac{dC}{dx} - \lambda C \tag{1}$$

+ Corresponding author. Tel: 822-2164-4373; fax: 822-2164-4865
jongscho@catholic.ac.kr

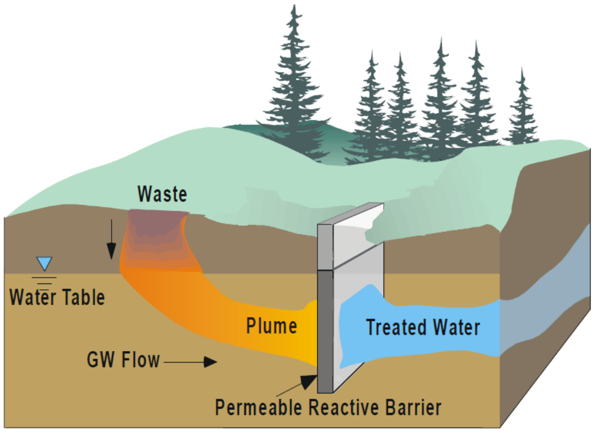

Fig. 1: A Schematic Diagram of Permeable Reactive Barrier

with boundary conditions,

at $x = 0, C=C_0$ (2)

at $x = \infty, C = 0$ (3)

Here D is the dispersivity, V the linear velocity, and λ is the first order reaction rate constant. Considering retardation of contaminant within groundwater flow through adsorption-desorption, the above equation can be modified to

$$0 = D^* \frac{d^2C}{dx^2} - V^* \frac{dC}{dx} - \lambda C^* \quad (4)$$

where D^* is D/R, V^* is V/R, $\lambda*$ is λ/R, and R is the retardation coefficient,. Let L be defined as a characteristic length to make the dimensionless space scale. For instance, it can be the distance between the source and the sensitive receptor for the application of monitored natural attenuation as a passive remediation measure of contaminated ground water.

For the permeable reactive barrier, the characteristic length becomes the thickness of the reactive wall. Dimensionless numbers are defined as follows;

$x^* = x/L,\ C^* = C/C_0$

Pe (Peclet number) = VL/D

Da_1 (the first Damköhler number) = $\lambda L/V$

Da_2 (the second Damköhler number) = $\lambda L^2/D = Pe \cdot Da_1$ when $Pe \neq 0$

The Damköhler number, Da, has the meaning of the ratio of the reaction rate to the transport rate (Damkőler, 1936; Jennings et al, 1984; Kuntz et al, 2009; Weber, 2001). The first Damköhler number is the ratio of reaction rate to the advection rate and the second Damköhler number is the ratio of the reaction rate to the dispersion rate. The Peclet number, Pe, is defined as the ratio of the advection rate to the dispersion rate. Here, for the case of the contaminant transport in groundwater, the dispersion is defined as the sum of molecular diffusion and mechanical dispersion, which is defined as hydrodynamic dispersion. In general, the mechanical dispersion dominates in groundwater so that the dispersivity can be expressed as $D = D_m = \alpha_L V$ (α_L, longitudinal dispersion coefficient). The Peclet number, Pe, becomes $VL/\alpha_L V = L/\alpha_L$, which means that the Peclet number is the ratio of the characteristic length, L, and the longitudinal dispersion coefficient, α_L, a physical property of hydrogeological media. The solution to the above equation can be obtained as follows;

$$C^*(x^*) = \exp\left[x^* \cdot \left(\frac{Pe}{2} - \sqrt{\frac{Pe^2}{4} + Pe \cdot Da_1}\right)\right] = \exp\left[x^* \cdot \left(\frac{Pe}{2} - \sqrt{\frac{Pe^2}{4} + Da_2}\right)\right] \quad (5)$$

At $x^* = 1$, C^* can be expressed as a function of Pe and Da_1 or Da_2 (Holzbecher, 2007).

$$C^*(1) = \exp\left[\frac{Pe}{2} - \sqrt{\frac{Pe^2}{4} + Pe \cdot Da_1}\right] = \exp\left[\frac{Pe}{2} - \sqrt{\frac{Pe^2}{4} + Da_2}\right] \quad (6)$$

It is possible to analyze the problem without considering the temporal and special scale with dimensionless numbers and to use the numbers to scale up laboratory experimental results to the field.

Case 1. No dispersion or very small case ($D \approx 0$) or plug-flow reactor: $Pe = \infty$

$$0 = -V\frac{dC}{dx} - \lambda C \quad (7)$$

with a boundary condition, at $x = 0$, $C=C_0$. The solution is

$$C(x) = \exp(-\lambda x / V) \quad (8)$$

In the dimensionless form, it becomes

$$C^*(x^*) = \exp\left(-x^* \cdot \frac{\lambda L}{V}\right) = \exp(-x^* \cdot Da_1) \quad (9)$$

Case 2. No advection and moleculardispersion only or completely mixed tank reactor; $Pe = 0$

$$C^*(x^*) = \exp\left(-x^* \cdot \sqrt{Da_2}\right) \quad (10)$$

3. Analysis of Permeable Reactive Barrier

At the Twin Cities Army Ammunition Plant (TCAAP) site in Minnesota, USA, trichloroethyle(TCE) contaminated groundwater was treated with a permeable reactive barrier filled with zero-valent iron powder. The system was designed based on the laboratory experimental data and analyzed with dimensionless numbers. The site conditions (US EPA, 2001) and reaction rates of TCE with zero-valent iron powder (US EPA, 1998) are in Table 1.

Table 1. Site conditions and reaction rates of TCE with zero-valent iron

Site Conditions		1st-order reaction rate constant, λ (hour^{-1})	
Linear flow velocity	3.19×10^{-2} m/hr	Column tests	0.7~1.44
Maximum concentration	25000 μg/L	Batch tests	$9.5 \times 10^{-3} \sim 3.25 \times 10^{-2}$
Target concnetration	5 μg/L		

Due to the high flow velocity, the thinness of the reactive barriers, and uniform homogeneous media in the reactive zone, the mechanical dispersion could be ignored that the Peclet number, *Pe,* becomes ∞ (no dispersion) and the solution of C^* could be obtained with the equation (9). Since C^* should be less than 2.0 x 10^{-4}, Da_I should be larger than 8.52. In case that the first order reaction rate was 0.7 $hour^{-1}$ as obtained in the column tests and the flow velocity was 3.19 x 10^{-2} m/hr, the thickness, *L*, should be larger than 0.39 m. If the first order reaction rate was 3.25 x 10^{-2} $hour^{-1}$ as the batch tests, the reactive barrier should be at least 8.4 m thick which was not feasible from the economical point.

4. Conclusions

The advection-dispersion-reaction equation for the contaminant fate and transport of contaminant in groundwater at steady state was solved with the dimensionless numbers. With those equations, TCE field test data from US EPA reports were analyzed and the performance of a permeable reactive barrier with zero-valent iron powder was simulated. The thickness of the reactive wall should satisfy the condition that Da_I should be larger than 9 to meet the target concentration with this passive remedial measure. Using the dimensionless numbers, it was quite simple to obtain the basic design parameter, the thickness of the reactive wall.

5. Acknowledgements

This research has been supported by the Korean Research Foundation (KRF) and the Romanian National Research and Development Institute of Cryogenic and Isotope Technologies.

6. References

[1] G. Damköhler. Einflusse der Stromung, Diffusion und des Warmeuberganges auf die Leistung von Reaktionsofen, *Zeitschrift Elektrochemie,* 1936, **42**(12): 846-862.

[2] E. Holzbecher. (2007), Environmental Modeling: Using MATLAB®, Chapter 5, pp. 87-100, Springer, Berlin, 2007.

[3] A. Jennings and D. Kirkner. Instantaneous equilibrium approximation analysis, *Journal of Hydraulic Engineering,* 1984, **110**(12): 1700-1717.

[4] D. Kuntz and P. Grathwohl. Comparison of steady-state and transient flow conditions on reactive transport of contaminants in the vadose soil zone, *Journal of Hydrology,* 2009, **369**: 225-233.

[5] US EPA. Permeable Reactive Barrier Technologies for Contaminant Remediation, *EPA/600/R-98/125*, OSWER, Washington, DC, 1998.

[6] US EPA. Evaluation of the Protocol for Natural Attenuation of Chlorinated Solvents: Case Study at the Twin Cities Army Ammunition Plant, *EPA/600/R-01/025*, OSWER, Washington, DC, 2001.

[7] W. Weber. Environmental Systems and Processes: *Principles, Modeling, and Design*, Chapter 11, p 337, John Wiley and Sons, New York, NY, 2001.