Apply THMC software to simulate the porosity reduction in a permeable reactive barrier-aquifer system

Presenter: Thi-Tuyet-Han Nguyen
Advisor: Prof. Jui-Sheng Chen
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Abstract

A permeable reactive barrier (PRB) involving zero-valent iron (ZVI) is an in-situ technique for treating groundwater contaminants. Chemical reactions occur inside the PRB, promoting secondary mineral precipitation and leading to a decrease in the porosity of the PRB. When the porosity is reduced, flow path reorientation, residence time changes, and bypassing occur. In this research, Thermal-Hydrology-Mechanic-Chemical (THMC) software was used to determine porosity reduction through flow modeling and the chemical reactions occurring within the PRB. According to the groundwater flow model, the PRB is more permeable than the neighboring aquifer materials, allowing water to pass through easily and preserving the groundwater's hydrogeology despite removing contaminants. The model results indicate that porosity loss is most significant at the entrance face (0.0138), followed by a fall and stabilization after 0.2 m at the PRB entrance. Aragonite, siderite, and ferrous hydroxide reduce porosity by more than 99%. This model highlights the relative effects of concentration by illustrating porosity losses for the high and low levels of bicarbonate and sulfate entering groundwater. The rate coefficient also influences porous reduction, while the anaerobic iron corrosion rate coefficient is highly sensitive to porous reduction due to iron corrosion influencing the formation of Fe^{2+}, OH^-, and the precipitation of $Fe(OH)_2$. The model indicates that the PRB is highly effective in reducing contaminants at the actual site. Therefore, the objective of this study is to use THMC to model the decrease of porosity in PRB, investigate the factors that should be considered when modeling porosity loss caused by mineral fouling in PRB, and analyze the reduction of porosity over time.

Keywords: Permeable reactive barrier (PRB), Zero-valent iron (ZVI), Thermal-Hydrology-Mechanic-Chemical (THMC), Porosity reduction.