Accepted Manuscript

Title: Transient reactive transport model for physico-chemical transformation by electrochemical reactive barriers

Authors: Shirin Hojabri, Ljiljana Rajic, Akram Alshawabkeh

PII: S0304-3894(18)30491-6
DOI: https://doi.org/10.1016/j.jhazmat.2018.06.051
Reference: HAZMAT 19488

To appear in: *Journal of Hazardous Materials*

Received date: 1-10-2017
Revised date: 22-6-2018
Accepted date: 23-6-2018

Transient reactive transport model for physico-chemical transformation by electrochemical reactive barriers

Shirin Hojabri, Ljiljana Rajic, Akram Alshawabkeh*

Civil and Environmental Engineering, Northeastern University, Boston, MA, 02115, USA

*Corresponding author: aalsha@coe.neu.edu; Tel: +1 617 373 3994

Research highlights:

- Theoretical one-dimensional model is developed for electrochemical transformation
- Chemical reaction model is combined with the transport and transformation
- Adopted a two-step iterative finite difference method to solve for the species
- Verification is provided for pH profiles
- Close correlation to experimental data; batch: R^2=0.99; flow-through: R^2=0.78

Abstract

A comprehensive model that integrates coupled effects of chemical, physical, and electrochemical processes, is necessary for design, analysis, and implementation of the electro-remediation of groundwater under flow conditions. A coupled system of equations to solve for transport and multiple reactions in an electrochemical reactor is numerically intensive due to highly stiff nature of reaction model formulation. In this study, the focus is to develop an efficient model for reactions associated with the transport and physico-chemical transformation in an electrochemical reactor. The model incorporates effects of transport mechanisms as well as chemical and electrochemical reactions. Model verification is provided for pH profiles under different electrolyte compositions in two sets of reactors; a batch and a flow-through reactor. The model is able to predict the concentration of species during the electrochemical remediation process with a close correlation to experimental data ($R^2=0.99$ for batch and $R^2=0.78$ for flow-through reactor.) Imposing polarity reversal to the system will cause fluctuation of pH, however, the trend stays the same as if no polarity were applied. Ultimately, volumetric charge flow is introduced as a unique parameter characterizing the electroremediation reactor for operating purposes.

Keywords: pH Modeling; Electrochemical Remediation; Groundwater Remediation; Physico-chemical Modeling

1. Introduction

Electrokinetic remediation is a valuable process for treatment of contaminated groundwater because of its environmental compatibility, versatility, energy efficiency, and low required maintenance [1–6]. The redox potential of the solution is altered during electrolysis, which can be manipulated to induce contaminant transformation and/or degradation reactions [7,8]. Electrochemical processes were initially investigated for oxidation of phenolic compounds in