



Multiphysics Implementation of Electrokinetic Remediation Models for Natural Soils and Porewaters



R. López-Vizcaíno^a, A. Yustres^{b,*}, M.J. León^b, C. Saez^c, P. Cañizares^c, M.A. Rodrigo^c, V. Navarro^b

^a Department of Chemical Engineering, Institute of Chemical & Environmental Technologies, University of Castilla-La Mancha, Campus Universitario s/n, 13071 Ciudad Real, Spain

^b Geoenvironmental Group, Civil Engineering School, University of Castilla-La Mancha, Avda. Camilo José Cela s/n, 13071 Ciudad Real, Spain

^c Department of Chemical Engineering, Faculty of Chemical Sciences & Technologies, University of Castilla-La Mancha, Campus Universitario s/n, 13071 Ciudad Real, Spain

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ABSTRACT

Models of electrokinetic soil remediation systems have been developed significantly in recent decades. A wide range of physicochemical phenomena occurs in this type of process, which makes it difficult to capture all of the system's complexity in a model. Therefore, existing models do not attempt to simulate the behaviour of the entire geochemical system of natural soils and their porewaters but rather focus on the pollutant compounds of interest. This paper proposes a conceptual and numerical model that includes geochemical speciation other than the phenomena that have been described by other authors. In addition, a comparative modelling exercise is performed with a composition of natural porewater and a simplified equivalent composition. The results show that the buffering system of carbonates affects the temporal evolution and spatial distribution of the pH. Because the pH controls many of the phenomena that occur during this type of remediation, simulations using realistic geochemical systems are critical.

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1. INTRODUCTION

Electrokinetic remediation (EKR) is a technology that has recently been applied in soil decontamination processes [1,2]. EKR technology allows contaminants of different ionic natures to be mobilised via various transport mechanisms that are generated by applying a low-intensity electric field between electrodes installed in the contaminated soil. This effect has generated significant interest in EKR technology in the field of in-situ soil decontamination. In addition, the energy requirements are generally low and can be supplied by renewable energy-based systems that are easily installed in any area to be decontaminated [3–5].

Electro-osmosis and electromigration are the main forms of mass transport that take place in the soil during an EKR process. The process of electro-osmosis causes the movement of water in the Debye layer, which is located along the surfaces of the soil particles. Generally, the soil surface charge is usually negative, so water that is capable of being mobilised through this mechanism

has high concentrations of positive counter ions, and electro-osmotic transport is generally directed towards cathodes [6–8]. Through the process of electromigration, it is possible to mobilise various ionic species present in the porewater that are electrically attracted to the oppositely charged electrodes. Among these ionic species are protons and hydroxyl ions generated in the electrochemical reactions of water electrolysis:



which occur on the surfaces of the anodes (Eq. (1)) and cathodes (Eq. (2)). The movement of these species produces an acidic pH front towards the cathodic electrodes and a basic pH front towards the anodic electrodes, whose velocity, in addition to the electromigration process, is significantly influenced by advective/diffusive processes and the soil's buffering capacity [9–11]. The pH fronts form a pronounced pH gradient in the soil that can favour the precipitation/solubilisation of species, adsorption processes, and ionic exchange between the soil and the porewater and,

* Corresponding author at: Civil Engineering School, University of Castilla-La Mancha, Avda. Camilo José Cela s/n, 13071 Ciudad Real, Spain.

E-mail address: angel.yustres@uclm.es (A. Yustres).

importantly, influence the chemical speciation of substances in the medium.

The coupling of these phenomena makes the design, analysis, and implementation of an EKR process in contaminated soil a very complex task. The development of mathematical models is necessary to characterise the interactions of the many physical, chemical, and electrochemical processes that occur simultaneously and therefore facilitate making predictions about the scaling of the technology. For this reason, the development of mathematical models of EKR processes has been important over the last 25 years. Shapiro et al. [7] and Shapiro and Probst [8] developed a one-dimensional mathematical model that considered the chemical equilibria of substances in the porewater, electrochemical reactions, diffusive and electro-osmotic transport, and ionic electromigration. The model was developed for the decontamination of a synthetic soil (kaolin) spiked with acetic acid and phenol. This model was improved by adding coupling complexation, adsorption and precipitation/dissolution processes by Jacobs et al. [12] and extended to a two-dimensional domain by Jacobs and Probst [13]. Other authors [14–16] developed a one-dimensional theoretical model that was applied to remove lead spiked in a mixture of kaolinite and sand, for which they estimated the pH profiles generated in the soil. Mascia et al. [17] proposed a similar model for the removal of cadmium. These models were generalised by Paz-García et al. [9] for application to soils contaminated with many metals. Other authors [18,19] have developed two-dimensional models that focused on the electrokinetic removal of metals and its application, in particular, to the remediation of soils contaminated with copper. Ribeiro et al. [20] developed a model adapted for the removal of organic pollutants and used atrazine as an example. A three-dimensional model has also been developed and used to simulate the electrokinetic transport of ions in soils under unsaturated conditions assuming that the lines of the electrical current in a soil during the application of an electrical gradient are analogous to the lines of a water current generated under a hydraulic gradient [21,22].

In this context, as proposed by Al-Hamdan & Reddy [23], many previous models utilise simplified geochemical systems because they generally contain fewer than 10 species, taking into account the reactants and products of the chemical and electrochemical reactions that can occur. This implies that the chemical speciation generated in the EKR process is quite limited and cannot faithfully reproduce the behaviour observed in real applications, where the composition of the natural porewater can be very complex. As mentioned above, chemical speciation is strongly related to the pH of the medium, which determines the extent to which many physico-chemical processes that directly affect the efficacy of an EKR process can be developed.

This study developed a model, M4EKR (Multiphysics for ElectroKinetic Remediation), that is applicable to electrokinetic remediation processes in natural unsaturated soils for the removal of ionic species present in porewater. An extended geochemical system with 34 species that are involved in 24 chemical equilibria resulting from the presence of the most common major ions in many natural groundwaters was studied. The model includes the transport of species due to electro-osmosis, electromigration, diffusion and advective flow.

After describing the proposed formulation, the scope of the model is illustrated by simulating an EKR process of a natural soil and porewater as opposed to the synthetic saturating waters that have been proposed in other studies. The results show the descriptive capacity of the proposed model. Finally, the same process is analysed assuming a reduced geochemical model. This exercise illustrates the limitations of simplified models that do not allow several relevant processes that occur in natural porewaters to be simulated. The results confirm the convenience of using

extended geochemical models to improve the characterisation and design of EKR processes in soils under natural conditions.

2. CONCEPTUAL AND NUMERICAL MODEL

The proposed model is a model of the reactive transport of solutes in partially saturated soils subjected to an external electrical gradient. For conceptual simplification, isothermal conditions (298.15 K over the entire domain) are assumed, and the gas pressure (GP) remains constant and equal to atmospheric pressure

2.1. Water transport

The balance of the mass of water per unit volume in a porous medium is given by the expression:

$$\frac{\partial m_w}{\partial t} + \nabla \cdot \mathbf{I}_w = 0 \quad (3)$$

where $\nabla \cdot$ is the divergence operator, \mathbf{I}_w is the mass flow of water ($\text{kg m}^{-2} \text{s}^{-1}$), and m_w is the mass of water per unit total volume (kg m^{-3}), which is defined as:

$$m_w = \phi \cdot S_r \cdot \rho_w \quad (4)$$

where ϕ is the porosity, ρ_w is the water density, and S_r is the degree of saturation of the soil. S_r is modelled using van Genuchten's retention curve [24], which is defined via the expression:

$$S_r = (1 + (\alpha_{VG} \cdot s)^{n_{VG}})^{-m_{VG}} \quad (5)$$

where α_{VG} , n_{VG} and m_{VG} are fitting parameters, and s is the matric suction, which is given by the difference between the gas pressure and liquid pressure, $P_G - P_L$.

The mass flow of water is defined by the sum of the hydraulic flux contributions (\mathbf{I}_w^h), which are estimated via Darcy's law, and the electro-osmotic flux (\mathbf{I}_w^{eo}), which is defined by the semi-empirical Helmholtz-Smoluchowski formulation [25]. Therefore, in the proposed model, we have:

$$\mathbf{I}_w = \mathbf{I}_w^h + \mathbf{I}_w^{eo} = \rho_w \cdot (\mathbf{q}_w^h + \mathbf{q}_w^{eo}) = \rho_w \cdot \mathbf{q}_w \quad (6)$$

$$\mathbf{q}_w^h = -K_e^h \cdot (\nabla P_L + g \cdot \rho_w \cdot \nabla z) \quad (7)$$

$$K_e^h = K_{sat}^h \cdot k_{rel}^h = K_{sat}^h \cdot S_r^3 \quad (8)$$

$$\mathbf{q}_w^{eo} = -K_e^{eo} \cdot \nabla E = -K_{sat}^{eo} \cdot S_r^3 \cdot \nabla E \quad (9)$$

where K_e^h is the effective hydraulic permeability of the soil, which is calculated by multiplying the saturated permeability (K_{sat}^h) by a relative permeability function. A Brooks and Corey-type power function was chosen for the relative permeability [26] with an exponent of 3. In addition, ∇ is the gradient differential operator, g is gravity, z is the vertical coordinate, E is the electric potential, K_e^{eo} is the effective electro-osmotic permeability of the soil, which is calculated using the same formulation employed in the calculation of K_e^h , and K_{sat}^{eo} is the saturated electro-osmotic permeability.

2.2. Chemical species transport

The proposed geochemical system includes a total of N species generated from the combination of M components selected among the species [27]. $M-2$ equilibrium equations of the total mass of

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