A reactive particle tracking model for a general flow field, and application to ISCO (In-Situ Chemical Oxidation)

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Introduction

One of the common approaches for the remediation of contaminated groundwater is the use of in situ chemical oxidation (ISCO). The method is based on injection of an oxidizing agent (e.g. permanganate) dissolved in water at wells [1]. The solution spreads within the aquifer and oxidizes the organic matter in the soil/rock and with the pollutant (e.g. TCE). The method was found to be effective at sites where the plume is relatively small. Also, it was found to be effective close to the contaminant source in the case of DNAPL lenses [2]. Usually, prior to ISCO operation, a significant number of pumping/injection wells are drilled at the site. During the operation, water is pumped from one of the pumping wells into a mixing tank, where it is mixed with the oxidizer. The solution is injected back into the aquifer at one of the injection wells. Typically the pumping, mixing and injection are done simultaneously. After some period of time (e.g. 1 hour), both the injection well and the pumping well are replaced. This is done in order to ensure a good mixing of the oxidizer and the pollutant, and to limit the displacement of the pollutant plume away from the injection well. The injection operation continues typically for a few days, and is followed by a periodic monitoring of the site for a few months. If the contaminant levels are still high, an additional ISCO operation may be needed.

In order to plan an optimal remediation process, and to reduce the cost of the process (especially reduce the cost of oxidizer used), a flow and transport model is needed. Such model describes the movement of groundwater, and the advection, dispersion, and reaction of the oxidizing agent and the pollutant. The reaction rate is described as a second order rate, i.e. dependent on the concentrations of the two substances. Therefore there is a coupling between the ADR (Advection-dispersion-reaction) equations of these components. A further complication of the mathematical problem may arise due to sorption of the contaminant and due to non-aqueous phase contaminant which may dissolve slowly into the groundwater.

Present numerical model (e.g. RT3D, [3]) can solve the for the temporal evolution of the concentrations of the contaminant and the oxidizer during the injection operation and in the months that follow it; however such models may be complex to operate and they require significant computational resources (both CPU time and memory). In addition, calibration of such models w.r.t to field observations is difficult [4,5]. An inherent problem in the present models is that they use an Eulerian formulation for calculating reaction rates, and thus miscalculate them at fronts. A partial remedy to this problem is to use fine grid resolution, but is very expensive in terms of computational resources. The alternative we propose is to use a Lagrangian approach, i.e. particle tracking (PT) models. In PT models, the concentration is represented by the density of a finite number of numerical particles (e.g. [6]). Present PT models can describe bimolecular reaction for pure diffusion [7,8] and for diffusion combined with linear shear advection [9]. In this research we develop the approach for the case of an arbitrary flow field, and apply the model to the case of a specific site in Israel, where ISCO was performed. We show that the model is a relatively simple and fast. At the same time, it can describe the important phenomena that take place during remediation. The model can predict the efficiency of multiple design alternatives and thus can serve to optimize ISCO.

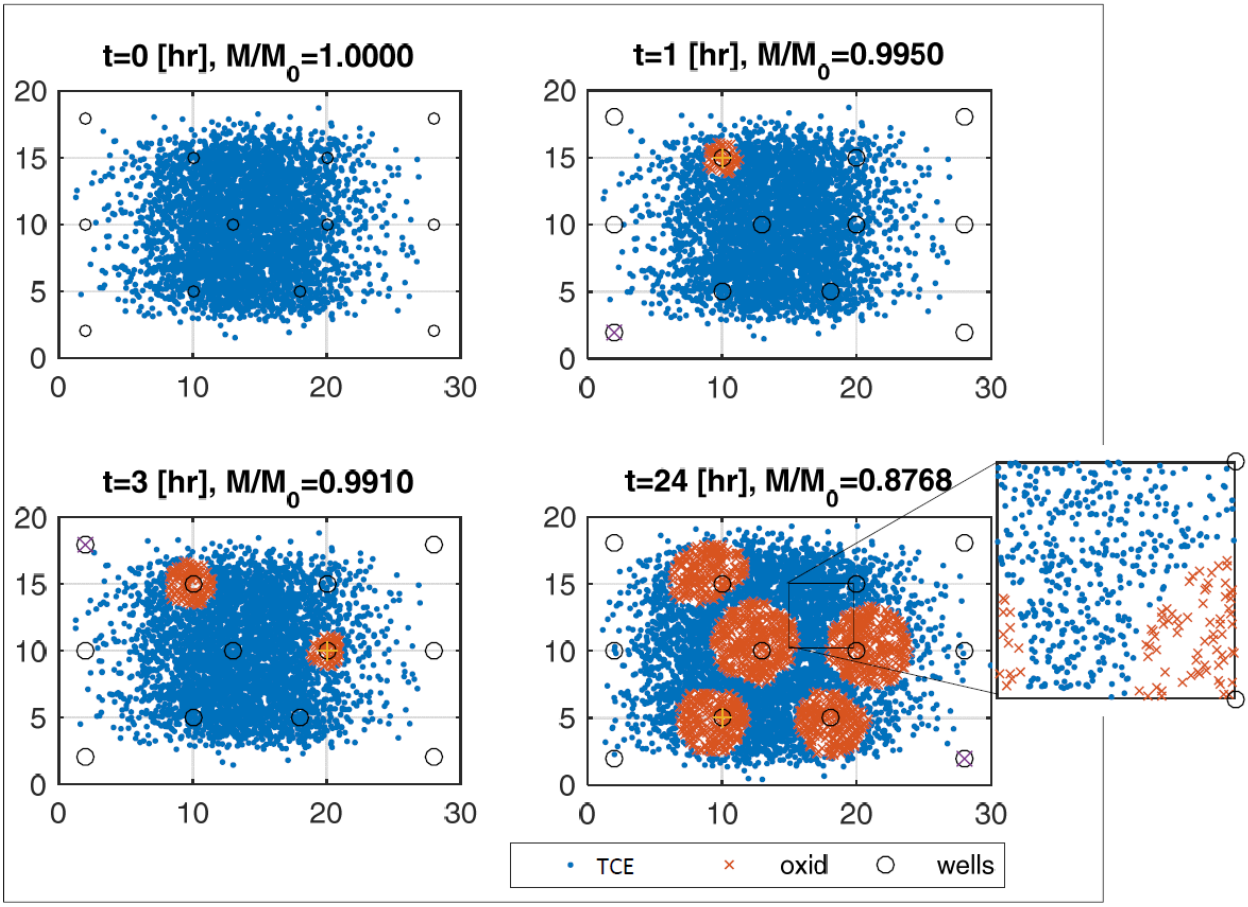

Figure 1: A synthetic example of a reactive PT simulation for 2D (top view) ISCO remediation

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