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Factors controlling BTEX and chlorinated solvents plume length under natural attenuation conditions

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Abstract

Natural attenuation is presently used at numerous sites where groundwater is contaminated. In order to simulate this attenuation, reactive transport models are often used but they are quite complex and depend on both physical and chemical conditions in the aquifer. As complex numerical models cannot be used to study all possible cases, we develop here analytical solutions to draw general conclusions. Our strategy, called MIKSS (Mixed Instantaneous and Kinetics Superposition Sequence), allows the calculation of the concentrations of all reacting substances in a plume. It is an extension of the superimposition principle that is able to treat the case of joint kinetics and instantaneous reactions. The basic equations have been extended to treat different reactions that occur in the plume core and at its fringe.

At first we consider one organic substance degraded under all oxidising conditions (toluene for instance). For this problem the size of the plume depends on the reduced source width and on the ratio of the organic substance concentration to the sum of the electron acceptors' concentrations. For several BTEX substances having different degradation behaviour the formulation is similar, but leads to quite different plume lengths for each substance. Contrary to the case of one substance, the plumes can be quite long and may not satisfy the target risk level.

For chlorinated solvents we developed a specific approach to take under consideration all reactions and particularly the competition for hydrogen. A formula is given to assess the size of the plume core, i.e. the zone with highly reducing conditions. The factors influencing the core length are the same as for BTEX (source width, dispersivity, organic carbon content). The size of the TCE plume is calculated from the plume core length and the kinetic constant of TCE degradation. Using assumptions of degradation constants for DCE and VC it is also possible to calculate the longitudinal concentration profile of these substances. The degradation of moderately substituted solvents under oxic conditions reduces the size of their plumes but under these

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conditions TCE becomes the major threat. Among the conditions studied in this paper, very few chlorinated solvents sites can lead to a negligible risk at an acceptable distance from the source.

Keywords: Natural attenuation; Modelling; BTEX; Chlorinated solvents; Analytical solutions

1. Introduction

In contaminated aquifers, organic pollutants are subjected to various degradation reactions mediated by bacteria (Rittmann, 2004). There is a strong need to understand these biodegradation reactions to manage contaminated sites. In fact, a general trend towards the use of bioremediation is evident at numerous sites. The use of natural attenuation assumes that natural processes occurring at a site will be efficient enough to prevent unacceptable risk at the target point. One can thus be able to predict the maximum concentration of a contaminant at a given distance from the source.

The major objectives of this paper are :

- the development of new analytical modelling techniques to predict core-controlled and fringe controlled degradation of BTEX and chlorinated solvents plumes,
- validation of the analytical model for different BTEX and chlorinated solvent release scenarios,
- identification of factors controlling the size of BTEX and chlorinated solvents plumes under natural attenuation conditions.

Other authors already addressed this question (Ham, 2004; Maier and Gratwohl, 2006), however they always considered a bimolecular reaction. Under natural attenuation simple bimolecular reactions are not widespread, because, most of time natural electron acceptors (EA) are used for several different reactions (Lu et al., 1999). The degradation of chlorinated solvents is far from bimolecular as it involves kinetic reactions and requires the presence of H_2 previously produced by other reactions (Semprini et al., 1995). We therefore developed a complete reactive approach that is able to treat both questions. Entirely explicit analytical solutions exist for simple 2D or 3D transport situations (Domenico, 1987) and integral forms are available for more complex cases (Tartakovsky, 2000; Park and Zhan, 2001). These transport solutions have been extended to treat simple instantaneous reactions with the help of the superposition principle (Borden et al., 1986). Koussis et al. (2002) showed that the superposition strategy is valid under most conditions, except during the early plume development.

Ham (2004) used the superposition approach to determine the size of BTEX plumes under the assumption of bimolecular instantaneous reactions. Maier and Gratwohl (2006) studied bimolecular reactions influenced by infiltration of clean water. However both studies did not differentiate the behaviour of each BTEX compound under different redox conditions, although it is known to occur at most sites (Barker et al., 1987; Borden et al., 1997; Lu et al., 1999). We thus extended the superposition principle to a series of reactions in order to determine the plume lengths of each BTEX substrate. There also exist analytical solutions for a series of substances that degrade in chain that is adequate for chlorinated solvents (Sun et al., 1999). These solutions are used for instance in the Biochlor model. However, it has been evidenced at numerous sites (Wiedemeier et al., 1999; An et al., 2004) that the most substituted chlorinated solvents are degraded only