# Aqueous Solubility and Chemical Reductive Remediation of Hexachloroethane and Hexachlorobutadiene

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Chlorinated organic compounds (COCs) have been widely used for many industrial purposes and are widespread distributed in the environment due to leaks and release from industrial sources. Hexachloroethane (HCA) and hexachlorobutadiene (HCBD) are among the more recalcitrant as they are more chemically stable and less soluble. They thus represent a major concern. Different remediation methods have been developed to clean up contaminated sites. Actions to carry out in order to prevent pollution risks require a knowledge of the outcome of COCs in the environment; this could be determined by modeling the various issues such as the aqueous release or the (bio)remediation processes of these pollutants. Physical properties, thermodynamic and kinetic parameters are required, and their determination constitutes the aim of the present study structured in two parts: the determination of the aqueous solubility of HCA and HCBD followed by the definition of the optimal conditions of their chemical reductive remediation.

The aqueous solubilities of HCA and HCBD have been measured independently as a function of temperature (between 12 and 45 °C) with the shake flask method. After establishment of the equilibrium, and centrifugation to separate the fine drops of dense non-aqueous phase, the supernatant was analyzed using standard GC/FID techniques. The operation was replicated from 4 to 6 for each condition. Experimental results show a non-linear evolution with temperature, with a minimum of solubility between 20 and 30 °C for both compounds. The temperature dependence equations of the thermodynamic functions concerning the solubility of the involved pollutants were determined in the range from 12 to 45°C, thanks of the method of Clarke and Glew (1966) using a Taylor series on the Van 't Hoff equation.

The chemical reductive remediation has been performed in batch reactor at 25 °C for HCA and HCBD dissolved in deionized water/methanol (99,9/0,1% v/v). Studied reductive agent is a suspension of micro-scale zero-valent iron particles (specific area $< 1$ m² g$^{-1}$) coated with palladium spots (5 % w/w) to enhanced iron reactivity. Particles are widespread in a slurry containing a water insoluble polyacid matrix which is used as a stabilizing agent to prevent aggregation of particles (Colombo et al., 2015). Palladium acts as a catalyst on the reduction reaction (Lowry and Reinhard, 1999; Zhang et al., 1998): it is responsible for the formation of very reactive hydrogen radicals. Dechlorination products have been identified and their concentration were measured by standard GC/MS and GC/FID techniques. A pseudo-first order kinetic law was determined for HCA, with a half-life of less than 30 min. The reaction undergoes a β-elimination pathway with the formation of PCE as the main reaction by-product. Only TCE and 1,1-DCE have been identified and quantified as other chlorinated by-products. For HCBD, results show a pseudo-first order kinetic law and a half-life of less than 20 min. No chlorinated by-products have been identified. The few numbers of by-products in both cases can be explained by the complete dissociation of C-Cl bond on the surface of palladium (Park et al., 1997). Work is in progress to model the influence of temperature on the reductive remediation.