

# Synthesis, Characterization, and Decontamination of TNT, RDX, and HMX Explosives in Wastewater by Zero-Valent Iron Nanoparticles

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## Abstract

This study has evaluated the efficiency of zero-valent iron nanoparticles (nZVI) for the remediation of soil and groundwater containing 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitroperhydro-1,3,5-triazine (RDX), and 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX). It was conducted via different treatment methods (batch experiments, column tests, and a permeable reactive barrier (PRB)) system. The combinative studies could be used to develop a more effective remediation technique. The chemical reactions that occurred upon mixing nZVI and contaminants provided the batch experiments extra harnessed power, leading to rapid reduction of the explosives. There was a decrease in the removal efficiency from 95% to less than 30% for the batch experiments owing to the lack of stirring facilities in the column test, PRB system and the interaction of the soil and explosives with nZVI. Kinetics studies indicated a more significant and rapid degradation of TNT than that of RDX and HMX, which was consistent with the lower activation energy of TNT. The X-ray spectroscopy results highlighted that during the reduction process, nZVI was transformed into core-shell structures with Fe(0) core and Fe<sub>3</sub>O<sub>4</sub> shell. High-performance liquid chromatography-mass spectrometry (HPLC/MS) tests depicted the decomposition of explosive contaminants into simple elements, such as carbon dioxide, nitrous oxide, and methane, over cleavage of the ring structure. When compared to other Fe species, the XANES analyses of the nZVI products were comparable to the Fe<sub>3</sub>O<sub>4</sub> standard. EXAFS results showed that after the reduction reaction of the nZVI and explosives, a core-shell structure consisting of the Fe(0) core and Fe<sub>3</sub>O<sub>4</sub> shell was created.

**Keywords** – Explosives, TNT/RDX/HMX, Zero-valent iron nanoparticles, Chemical reduction, Decontamination

