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Nitriding of nZVI as a novel means to improve its selectivity for trichloroethylene remediation

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Nanoscale zerovalent iron (nZVI) particles represent an attractive material for the in situ remediation of chlorinated organic pollutants such as trichloroethylene (TCE). Despite many promising laboratory and field studies conducted in the past two decades, the field-scale application of nZVI is still limited mainly due to low electron selectivity leading to fast particle corrosion and short longevity. This drawback, accompanied by the need to frequently repeat the injection of nZVI, significantly increases the treatment costs.

This study aimed to investigate nitriding as a novel means to improve nZVI performance [1]. Two different types of nanoparticles were synthesized by passing gaseous NH_3/N_2 mixtures over pristine nZVI at elevated temperatures. Nitrogen diffused throughout the entire volume of the nZVI particles, forming distinct bulk Fe_xN phases, mostly face-centered cubic (γ'-Fe_4N) and hexagonal close-packed (ε-$Fe_{2-3}N$) arrangements. The Fe_xN particles were thoroughly characterized using a broad range of techniques, such as XRD, XPS, HRTEM including EDX elemental mapping, and Mössbauer spectroscopy. Nitriding was found to increase the particles' hydrophobicity and surface availability of iron in reduced forms. The reactivity of both fresh and aged Fe_xN particles was assessed in batch experiments with TCE. The dechlorination mechanism was further studied by a combination of DFT calculations and experiments.

The two types of Fe_xN nanoparticles showed about 20- and 5-fold increase in the TCE dechlorination rate and about 3-fold decline in the hydrogen evolution rate compared with pristine nZVI. The first TCE dechlorination step was predicted by DFT with a relatively low energy barrier of 27.0 kJ mol^{-1}. TCE dechlorination experiments with aged particles showed that the Fe_xN nanoparticles containing mostly the γ'-Fe_4N phase retained high reactivity even after three months of aging. This study demonstrates that nitriding represents a promising strategy to improve nZVI performance.

References

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