

Ph.D. DISSERTATION DEFENSE

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Date: Tuesday, August 19th, 2025

Time/Location: 1:00 p.m. /https://stevens.zoom.us/j/93009158615?from=addon

Title: Degradation of high-energy compounds using nZVI-biochar

Chairperson: Dr. Dibyendu "Dibs" Sarkar, Department of Civil, environmental,

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Committee Members: Dr. Christos Christodoulatos, Department of Civil, Environmental,

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ABSTRACT

Nitro compounds are widely used in pharmaceutical, mining, and defense industries. Their high solubility, chemical stability, and resistance to degradation contribute to their persistence in industrial wastewater. This poses significant environmental and public health risks. This dissertation evaluates biochar-supported nanoscale zero-valent iron (nZVI-BC) composites as a sustainable treatment technology for nitro compound removal from aqueous systems. Nitroglycerin (NG), commonly found in both pharmaceutical and munitions wastewater, was selected as a model compound.

The first phase of the study investigated the effect of operational parameters on NG degradation using nZVI-BC. Variables included solution pH, iron-to-biochar ratio, reagent dose, and NG concentration. Results showed over 99% NG removal within 30 minutes under optimal conditions. The composite was effective across a broad pH range (3-11) and remained reactive under open-air conditions. Byproducts were quantified, and carbon and nitrogen mass balances were constructed. Reductive degradation was confirmed as the primary removal mechanism, with glycerol and ammonium, two benign products, as major end-products.

Kinetic modeling was used to describe degradation behavior. Two reaction pathways were evaluated. A model involving simultaneous dissociation of multiple nitro groups better matched experimental data than the traditional stepwise reduction model. Pseudo-first-order rate constants were derived and analyzed. Degradation rate was positively correlated with iron and biochar content and negatively affected by higher pH and pyrolysis temperature.

The influence of synthesis conditions on nZVI-BC performance was examined in the next phase. Biochars were produced from rice hull and vetiver root at different pyrolysis temperatures and durations. nZVI-BC was synthesized via chemical reduction. Materials were characterized and evaluated for NG removal. Two alternative synthesis methods, carbothermal reduction and copyrolysis, assessed. These methods produced iron oxide-based materials with lower removal efficiency.

This research offers mechanistic insight into nitro compound degradation using a rapid, waste-derived treatment approach. The findings contribute to the development of scalable, low-impact technologies for remediating industrial wastewater.