STEVENS INSTITUTE OF TECHNOLOGY 1870

Ph.D. DISSERTATION DEFENSE

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Title:	Zero Valent Magnesium (ZVMg) Treatment of Energetic Compounds 2,4-Dinitroanisole (DNAN) and Nitroglycerin (NG): A study of Kinetics and Mechanism in Both Fluidized-Bed and Stirred-Tank Reactors
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ABSTRACT

Currently, Energetic materials (EMs) have been wildly used and cause extensive pollution. Since their chemical nature is resistant to oxidation degradation, reductive degradation pathway is mostly selected by current study. Moreover, increasing accumulation of waste magnesium from metal factories poses environmental challenges. This dissertation investigates the reductive degradation of EMs using waste magnesium; in order to improve the efficiency of magnesium, glacial acetic acid was employed to remove passivation layer of magnesium.

To identify the optimal conditions for the degradation of energetic materials (EMs), various solid–liquid ratios (S/L) ranging from 0.5% to 10% and initial glacial acetic acid concentrations between 0.1% and 3% were evaluated in a stirred-tank reactor. Across all experiments, nitroglycerin (NG) removal ranged from 11% to 100% within 20 minutes. Additionally, Mg^{2+} concentrations were analyzed to elucidate the mechanisms governing EMs reduction. The results indicated that NG reductive degradation was driven by electron flux generated through the reaction between zero-valent magnesium (ZVMg) and acetic acid. A comprehensive kinetic model was subsequently developed and globally fitted to experimental NG and Mg^{2+} data by solving a system of ordinary differential equations (ODEs). The model successfully reproduced the observed trends in NG and Mg^{2+} concentrations, achieving a coefficient of determination (R^2) greater than 98%. Overall, the kinetic model provides a practical framework for describing and predicting NG removal under varying conditions in a ZVMg-catalyzed acetic acid system.

Building on the demonstrated effectiveness of the ZVMg-catalyzed acetic acid system for NG removal, a pilot-scale fluidized bed reactor (FBR) using magnesium and glacial acetic acid was developed for the degradation of DNAN. To optimize operating conditions—distinct from the stirred-tank reactor (STR) setup—various acetic acid dosages and superficial liquid velocities were tested under a constant solid–liquid ratio. DNAN removal was only 4% in the absence of acetic acid, whereas more than 94% removal was achieved with 2% acetic acid. Overall, the FBR attained higher DNAN removal efficiencies with lower acid requirements and shorter hydraulic retention times compared to the STR. Additionally, a modified computational fluid dynamics (CFD) model was applied to evaluate the system from hydrodynamic and chemical perspectives. Simulated pressure drops and particle motion in both reactors closely matched the experimental observations. Chemical-reaction simulations further revealed that the uniform distribution of radical species within the aqueous phase resulted from the fluidized bed's ability to create an optimal particle mixing zone.