

**Reactions of Chlorinated Ethenes with Surface-Sulfided Iron Materials:  
Reactivity Enhancement and Inhibition Effects**

Syful Islam<sup>1,^</sup>, Yanlai Han<sup>1,^,#</sup>, Weile Yan<sup>1,2\*</sup>

<sup>1</sup>Department of Civil, Environmental and Construction Engineering, Texas Tech University,  
Texas, United States

<sup>2</sup>Department of Civil and Environmental Engineering, University of Massachusetts Lowell,  
Massachusetts, United States

<sup>^</sup> with equal contribution

<sup>#</sup> Current affiliation: U.S. EPA National Exposure Research Laboratory

<sup>\*</sup> Corresponding author. Tel: (978)-934-2256

Email address: [weile\\_yan@uml.edu](mailto:weile_yan@uml.edu)

## Chemicals

Cu(II), Ni(II), and Mn(II) solutions were prepared from the respective salts: copper chloride dihydrate (Alfa Aesar), nickel (II) acetate tetrahydrate (Aldrich), and manganese chloride tetrahydrate (Fisher). TCE (99.5%), trans-dichloroethene (trans-DCE, 98%), cis- dichloroethene (cis-DCE, 97%), and 1,1- dichloroethene (1,1-DCE, 99%) were purchased from Aldrich. Vinyl chloride (VC, 1000 µg/mL in methanol) was purchased from AccuStandard. Iron (III) chloride hexahydrate ( $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ , 97.0%-102.0%) and sodium sulfide nonahydrate ( $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$ , 98%) were from Alfa Aesar. Sodium thiosulfate anhydrous ( $\text{Na}_2\text{S}_2\text{O}_3$ , 99.6%), sodium dithionite ( $\text{Na}_2\text{S}_2\text{O}_4$ , 99%) and ethanol (95%) were obtained from Fisher Scientific. Paraffin mixture (1000 ppm of methane, ethane, propane, butane, pentane, and hexane in helium) and olefin mixture (ca. 1000 ppm of ethene, propylene, 1-butene, 1-pentene, and 1-hexene in helium) were obtained from Matheson Tri-Gas and were used as calibration standards. Deoxygenated deionized-distilled water (DDI), prepared by purging DDI with  $\text{N}_2$  for 30 min, was used in all procedures including particle synthesis and TCE dechlorination experiments.

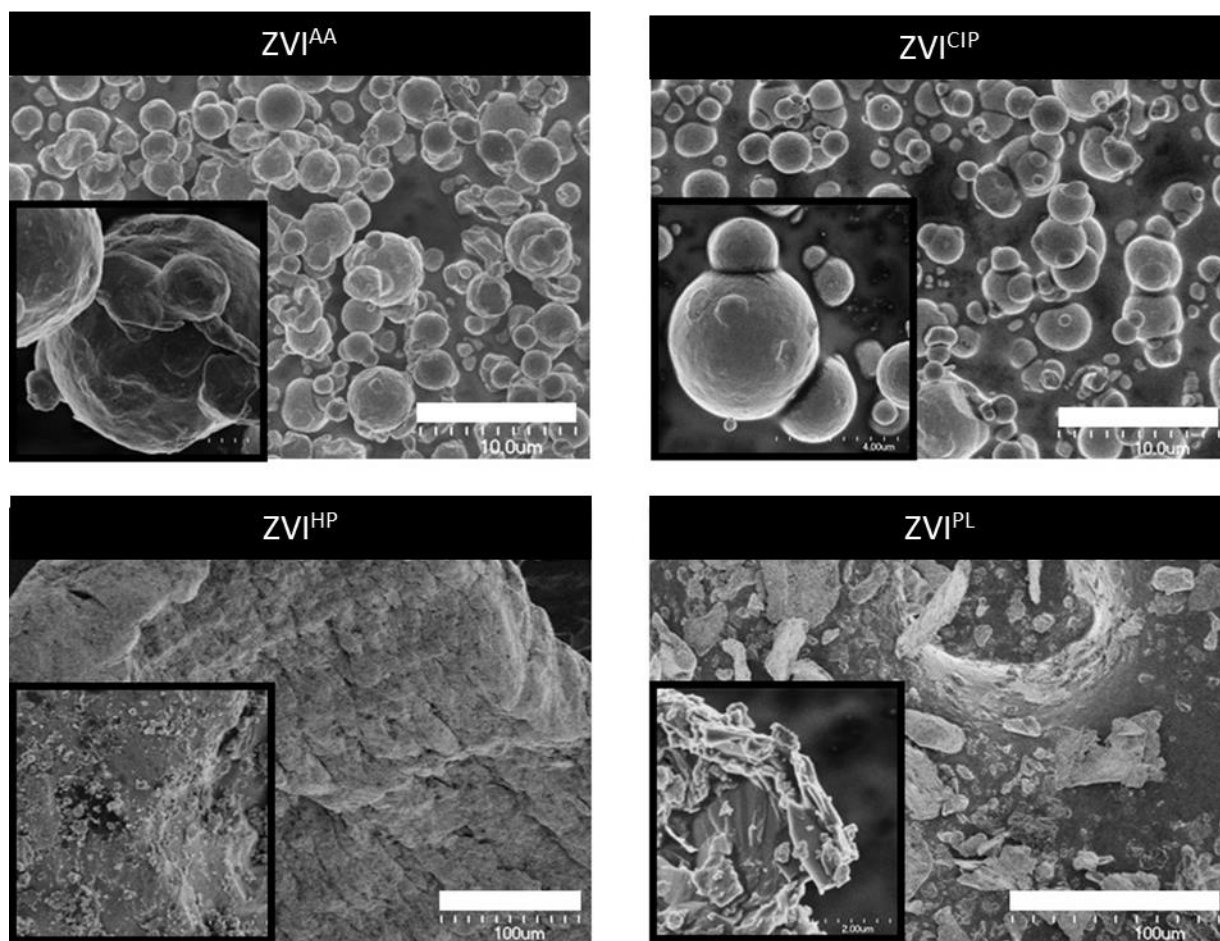


Figure S1. SEM micrographs of various ZVI materials evaluated in this study. The insets show magnified views of the surface details of the ZVI particles.

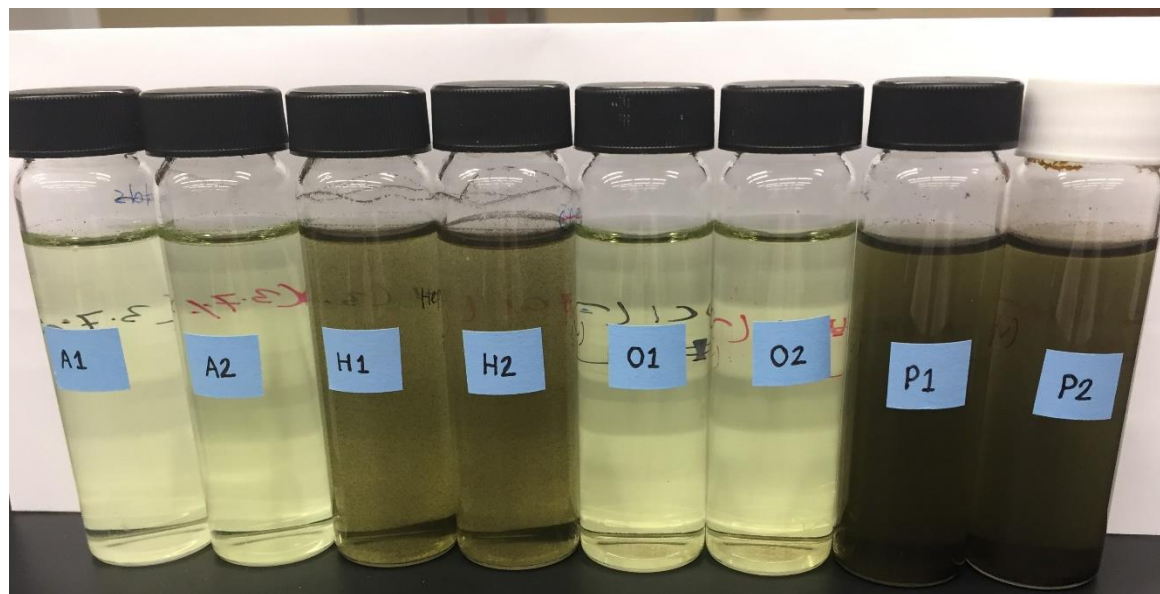


Figure S2. Visual appearance of ZVI suspensions after digestion in HCl solution (5.6% v/v) for 3 days. Bottles labelled with “A”, “H”, “O” and “P” are replicate suspensions of  $ZVI^{AA}$ ,  $ZVI^{HP}$ ,  $ZVI^{CIP}$ , and  $ZVI^{PL}$ , respectively.

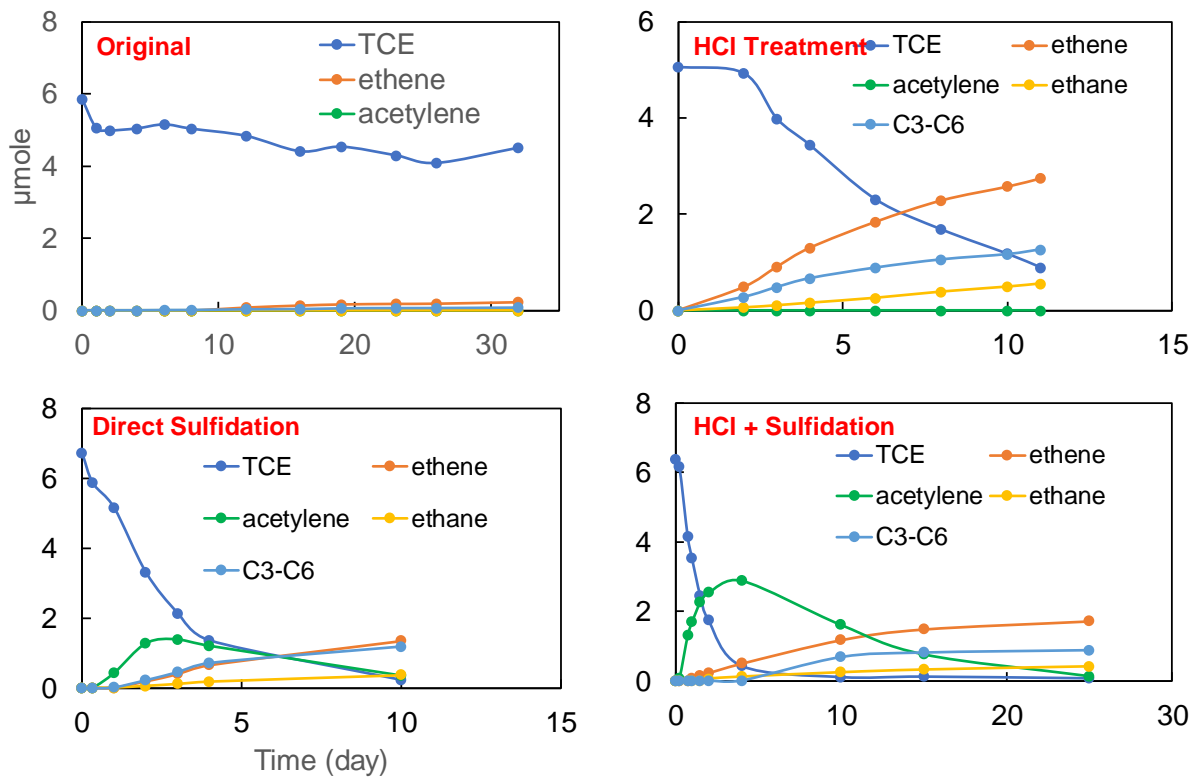
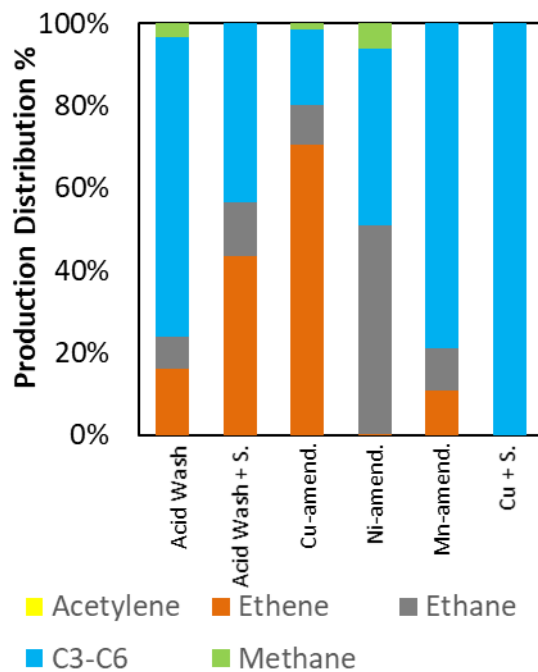


Figure S3. Products of TCE dechlorination by as-received and treated ZVI<sup>PL</sup>. TCE initial concentration was 25 mg/L. Fe loading was 10 g/L.

(a)



(b)

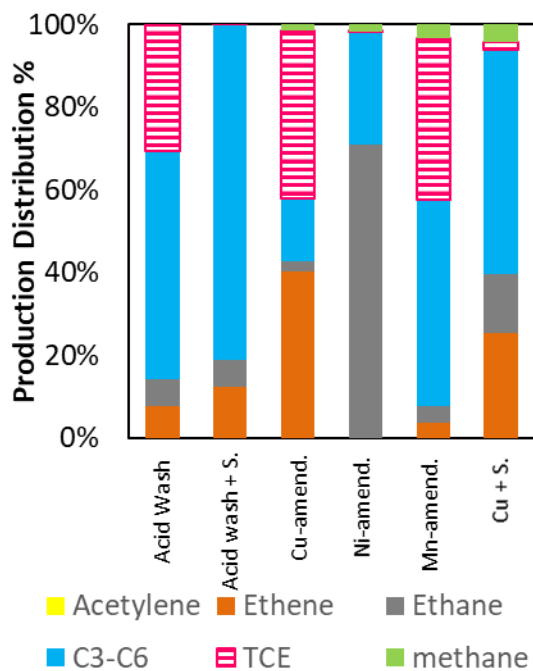


Figure S4. Distribution of products formed during (a) *cis*-DCE and (b) PCE degradation by acid-washed, sulfided, and metal-amended ZVI<sup>CIP</sup>.