Supporting Information

for

Catalytic Converters for Water Treatment

Kimberly N. Heck,1,2 Sergi Garcia-Segura,1,3 Paul Westerhoff,1,3 Michael S. Wong1,2,4,5,6*

1 Nanotechnology Enabled Water Treatment (NEWT) Center, 6100 Main St., Houston, TX, 77005
2 Department of Chemical & Biomolecular Engineering, Rice University, Houston, TX, 77005
3 School for Sustainable Engineering and the Built Environment, Arizona State University, Tempe, AZ, 85281
4 Department of Civil & Environmental Engineering, 5 Chemistry, 6 Materials Science & NanoEngineering, Rice University, Houston, TX, 77005

*Corresponding author: mswong@rice.edu
Calculation of Catalyst Cost

The modules will likely be flow modules, similar to packed bed reactor. For a first-order (or pseudo-first order) reaction, the design equation for a packed-bed reactor is given by:

\[ W = \frac{\nu}{k_{cat}} \ln \left( \frac{C_{NO3,o}}{C_{NO3}} \right) \]

where \( W \) is the weight of catalyst required, \( \nu \) is the volumetric flowrate, \( k_{cat} \) is the pseudo-first order rate constant normalized by catalyst concentration, \( C_{NO3,o} \) is the initial concentration of nitrate and \( C_{NO3} \) is the concentration of nitrate at the outlet.

Using a flowrate of 80 gal/day\(^1\) (0.21 L min\(^{-1}\)), kinetic constants of a Al\(_2\)O\(_3\) supported 1 wt% Pd and 0.13% In catalyst (0.23 L g\(_{\text{total catalyst}}\)\(^{-1}\) min\(^{-1}\)),\(^2\) and wishing to reduce a "high" concentration of 10 mg/L NO\(_3^-\) to 1 mg/L (at which NO\(_3^-\) ceases to have health effects),\(^3\) we calculated that 2.11 g of total catalyst would be required, consisting of 0.211 g of Pd and 0.0027 g of In. Spot checked on January 9, 2019, the price of Pd and In were $42.8\(^4\) and $0.40\(^5\) per gram, respectively, for a total catalyst (capital) cost of $0.91.

Calculation of Hydrogen Cost

We recently calculated the cost of electrolytically generating hydrogen to treat nitrate contaminated water for ion exchange brine regeneration. With an electricity rate of $0.08 kWH, 100% selectivity to N\(_2\) and 10% H\(_2\) utilization efficiency, the cost to treat 1 m\(^3\) of 100 mg/L NO\(_3^-\) contaminated water was $1.8. To 10\(^x\) less concentrated nitrate typical of household waters, the hydrogen requirement drops substantially, resulting in a cost reduction to $0.0018/gallon