Oxidative Treatment of Industrial Wastewater: Development of Novel catalysts and technology Evaluation

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Motivation for Research

- Pulp and paper mills and settling ponds can generate large quantities of fresh water.
- A simple, inexpensive, and scalable technology is needed to treat organic and inorganic compounds.
- The focus of this project is to develop improved and cost-effective technologies for this purpose.

Scope of Project

- Catalyst Development
  - Develop a catalyst that catalyzes the oxidation of ferulic acid (model lignin compound) in the presence of air at mild temperatures and pressures.
  - The resulting wastewater is biologically (i.e. lignin) and biologically (i.e. lignin) toxic to the environment.
- Kinetic Modeling
  - Develop a kinetic model that sufficiently describes the behavior of the system.
- Reactor/Process Modeling
  - Develop a reactor model to describe the behavior of the process on the industrial scale in order to estimate an overall mass balance, energy requirements, and the economics of the process.

Catalyst Development and Experimental Work

- What was studied?
  - A model lignin compound was chosen as ferulic acid (Figure 1).
  - Ferulic acid was reacted in the presence of air with (Catalytic Wet Oxidation, CWO) and without (Wet Oxidation, WO) the developed catalyst (Cu/CuO).

- Experimental Work (continued)

  - The resulting wastewater is biologically (i.e. lignin) toxic to the environment.
  - TOC versus time data was collected throughout each experiment held at constant RPM from 250-1200 RPM (Figure 3A).
  - TOC versus time data was collected throughout each experiment held at constant temperature from 90-1050C at 1 MPa pressure (Figure 3).
  - A mixing study was performed to ensure mass transfer limitations of oxygen and water were not an issue.
  - A temperature study was performed to see the effect of temperature on the WO and CWO system.

  - Total organic carbon (TOC) data was collected over the time span of each experiment.

  - The lumped kinetic models fit experimental data better than the simple TOC based model in Figure 4.
  - Fitting k-values for the 4 parameter lumped kinetic model were more difficult due to oversimplification of k-values (i.e. lumped [cat] terms inside k’ values).
  - The lumped models did not show asymptotic behavior with data, which is problematic when describing behavior at higher time values.

Kinetic Modeling

- What is involved in kinetic Modeling?
  - 1) Make assumptions that simplify complex chemistry; 2) derive rate equations to describe behavior of assumed chemistry; and 3) determine the kinetic parameters from gathered experimental data.

- 3 main kinetic models investigated

  - Simple TOC based Model: All organic species are approximated by a single parameter (Figure 4).
  - 2 Parameter Lumpred Model*: Only intermediates are lumped together (non-catalytic) (Figure 4).
  - 4 Parameter Lumpred Model*: Only intermediates are lumped together (both catalytic/non-catalytic) (Figure 4).


Conclusions

- The lumped kinetic models showed better agreement than a simple TOC based model in Figure 4.
- Fitting k-values for the 4 parameter lumped kinetic model were more difficult due to oversimplification of k-values (i.e. lumped [cat] terms inside k’ values).
- The lumped models did not show asymptotic behavior with data, which is problematic when describing behavior at higher time values.