Nano-Enabled Catalysts for the Commercially Viable Production of H₂O₂

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September 26, 2007
Headwaters Technology Development Principle

- Develop future generation technology not only creates value for industry, but also benefits the environment and human health.
Green Projects at Headwaters

- Waste coal conversion into solid alternative fuel
- Waste pyrolysis oil from ethylene cracking to value-added chemicals - BTX, gasoline and diesel
- NOx removal
- Sulfur removal
- Mercury removal
- Direct synthesis of hydrogen peroxide
Hydrogen Peroxide

- A environmentally friendly molecule $\text{H}_2\text{O}_2$

Upon decomposition, it releases water and oxygen:

$$\text{H}_2\text{O}_2 = \text{H}_2\text{O} + \frac{1}{2}\text{O}_2$$
Current Hydrogen Peroxide Applications

- 2006 global hydrogen peroxide use as oxidant ~ 2 million tons
- 2005 global hydrogen peroxide production ~ 3.5 million tons

![Pie chart showing the applications of hydrogen peroxide: 60% Bleaching Agent, 22% Manufacturing Chemicals, 18% Environmental, Textile, Mining]

Demand for H₂O₂ has grown significantly in recent years. But high cost slowed down its replacement of chlorinated oxidants which have serious environmental impacts.
A new process to make $\text{H}_2\text{O}_2$

$$\text{H}_2 + \text{O}_2 = \text{H}_2\text{O}_2$$

- Clean process
- Water or Alcohol as working solution
- No waste generated
- Water is the only by-product

Hundreds of million dollars invested by chemical companies like Dupont, BASF, Dow, Mitsubishi, Solvey, Degussa, etc.
Direct Synthesis of $\text{H}_2\text{O}_2$

> 100 patents between 1980s and 1990s

<table>
<thead>
<tr>
<th>Company</th>
<th>Number of Patent</th>
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<tbody>
<tr>
<td>Air Products</td>
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<td>21</td>
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## HTI’s Results vs. Patented Data

<table>
<thead>
<tr>
<th>Patent Number</th>
<th>Assignee</th>
<th>H\textsubscript{2} in Feed (vol.%)</th>
<th>H\textsubscript{2}O\textsubscript{2} Concentration (wt%)</th>
<th>H\textsubscript{2}O\textsubscript{2} Selectivity (%)</th>
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<td>Continuous Production</td>
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</tbody>
</table>
NxCat Nanotechnology is the Key to HTI’s Process

1) Controlled nanoparticle size.
Maximum productivity at lowest cost

2) Controlled nanoparticle composition.
Reduced bi-products and waste

3) Catalyst surface structure.
≈100% selectivity / “Green Chemistry”

4) Controlled nanoparticle dispersion.
High efficiency and yield

5) Anchored nanoparticles.
Long life, lower cost catalyst
NxCat Catalyst Features

1. 4 nm particles -- 2 nm makes water!!
2. Uniform metal alloy particles -- 50:1
3. 110 crystal structure ≈100% selectivity
4. Highly dispersed low metal loading -- 10x more productive than competition
5. Anchored particles >3 year life

DSHP Catalyst

NxCat Nanotechnology is the Key to HTI’s Process
Conventional vs. Direct Synthesis Process

**Conventional H$_2$O$_2$ Process**

- Hydrogenation
- Oxidation
- Extraction
- Distillation

**Direct Synthesis H$_2$O$_2$**

- Hydrogen + Oxygen
- Chemical Intermediate Hydrogen Peroxide in Solvent

NxCat nanotechnology enables simple manufacturing process with up to 50% lower capital cost and 20% lower H$_2$O$_2$ cost.
Direct Synthesis of Hydrogen Peroxide Milestones

- Sept. 2004: Joint venture with Degussa
- Mar. 2005: Pilot plant operation
- Oct. 2005: Commercial demonstration plant contraction started
- Oct. 2006: Commercial demonstration plant operation
- 2007: Data collection for design of 200,000-ton commercial plant
- 2008: Commercial plant construction scheduled to start
- 2010 and beyond: every other year a new 200,000-ton plant to be built

Commercial Demonstration Plant
Hanau Wolfgang, Germany
Conclusions

- Direct Synthesis is an environmental friendly process
  - Reduce energy consumption by a simple and more efficient process.
  - Low cost $\text{H}_2\text{O}_2$ has potential to replace chlorinated oxidants that have serious environmental impacts.
- Nanotechnology is the key to enable the new cutting edge process for commercially viable production
Acknowledgements

- Environmental Protection Agency
- American Chemical Society
- National Science Foundation
- Department of Energy
- Evonik Degussa
- HTI Team for Direct Synthesis of H₂O₂
Direct Synthesis of Hydrogen Peroxide Team
Presidential Green Chemistry Challenge Award