DOE Chemical Hydrogen Storage Center of Excellence

Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides

Project ID# STP11

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This presentation does not contain any proprietary or confidential information

Project Overview

Time Line

- Project start date
  - Fiscal Year 2005
- Project end date
  - Fiscal Year 2009
- Percent complete
  - New start

Barriers

- High cost and energy requirements for regenerating spent fuel from irreversible chemical H_2 storage systems

Budget ($)

Year	DOE	ROH	Total
FY05 (Actual)	275,000	124,000	399,000
Total (Requested)	1,768,202	821,992	2,590,194

New project. No funding received in 2004. ROH:DOE split = 31:69

Partners

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Los Alamos National Laboratory 1943 - 2003 Ideas That Change the World

Millennium Cell

PennState 1855

Pacific Northwest National Laboratory Operated by Battelle for the U.S. Department of Energy

BORAX

The University of Alabama

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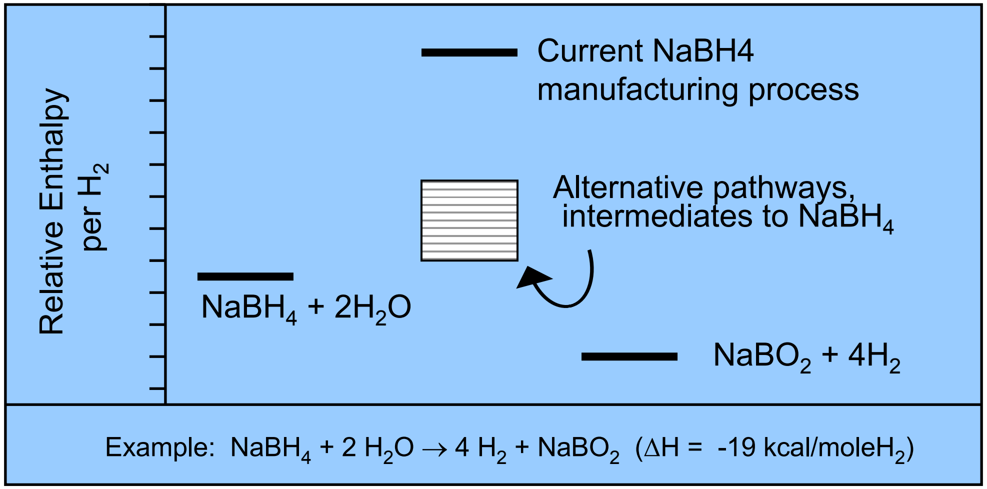
Objectives

- Define and evaluate novel chemistries and processes to produce chemical hydrides for hydrogen storage
- Focus on Tier 1 Research :
  - Conversion of B-O to B-H in spent fuel
  - Optimize energy efficiency and minimize cost



Objectives (continued)

- Leverage our experience and expertise across all 3 Center Tiers
  - Identify opportunities to improve the technology of the other Center participants
  - Ensure the success of the Center

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ROH Contributions to the COE

- Who are we ?
  - Oldest and largest producer of $NaBH_4$ worldwide
  - Two world-class ISO 9002-certified production plants
  - Allied Partner with DOE (2003)
  - Listed Among America's Top 5 Most Admired Chemical Companies (Fortune Magazine)
- What we bring to the Center :
  - Extensive intellectual property portfolio, including technology, technical information and data on $NaBH_4$ and other chemical hydrides (50+ years)
  - Expertise in
    - Chemical and engineering assessment capabilities for chemical processes
    - New product formulation, application development, and commercialization
    - Understanding customer and market needs
  - Unparalleled manufacturing, supply chain, logistics, distribution expertise
  - Expertise in Environmental, Health, and Safety
    - American Chemistry Council, AIChE CCPS involvement
    - OSHA Star VPP Award (Elma, WA $NaBH_4$ plant)

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Approach – Four Main Tasks

- Data Mining and Development of Work Processes
- Engineering-Guided Research of Chemical Borate Reduction Routes
- Complexation and Reduction of Borates
- Electrochemical Reduction of Borates to Borohydride

Task 1 – Data Mining and Development of Work Processes

- Goals
  - Compile existing technical information to identify viable pathways
  - Develop technical targets, criteria and metrics to ensure consistent evaluation of options
  - Draw upon data and reports in US Borax, Redstone Arsenal, US Navy Fuel Program files to identify possible options
- Partners
  - LANL, PNNL, Millennium Cell, US Borax, Pennsylvania State University

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Task 2 – Engineering Guided Research of Chemical Borate Reduction Routes

- Goals
  - Conduct detailed engineering assessment of as many chemical borate reduction routes as possible, against established metrics
  - Reduce options : identify routes that do not meet established criteria
  - Identify leading routes to be pursued experimentally by Center participants
- Partners
  - LANL, PNNL, Pennsylvania State University, Millennium Cell

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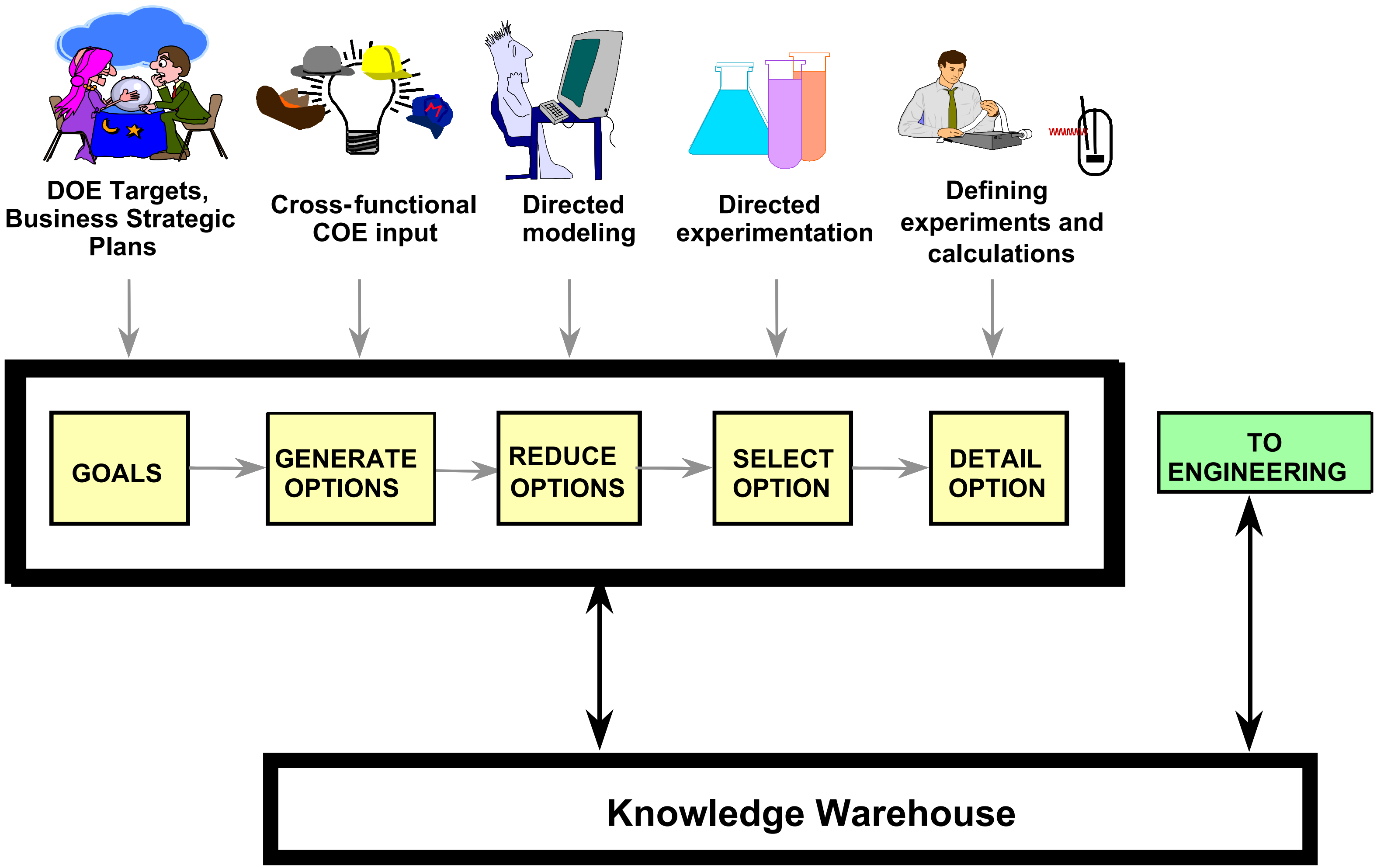
Engineering-Guided Research of Chemical Borate Reduction Routes



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Goal Deliberation

- Define Goals and Objectives
- Boundaries and Assumptions
- Evaluation Criteria/Metrics
  - Cost
  - Energy Efficiency
  - Life Cycle Inventory and Analysis
  - Economics
  - DOE Targets
  - Environmental, Health, Safety and Sustainable Development

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Options Generation

- Identify potential routes to produce $NaBH_4$ and other chemical hydrogen storage materials
  - Evaluate prior data to identify leading routes/systems
  - Compile and organize concepts
  - Brainstorm additional processing options
- Information Collection
  - Strategy
  - Sharing of relevant literature
  - Data-mining

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Options Reduction

- Develop options matrix
- Define basic reaction envelopes and flowsheets
- Conduct preliminary technical and economic viability analysis
- Identify information gaps
- Establish experimental/computational needs (key data required for validation)
- Select leading options

Option Selection and Development

- Complete experimental/computational viability studies (with Center)
- Refine flowsheets based
  - on updated energy requirements
  - raw material and wastes
  - Environmental, Health, Safety, and Sustainable Development considerations
- Define optimized process
- Engineering/economic analysis with Life Cycle Analysis
- Conceptual and pilot plant designs
- Process scaleup

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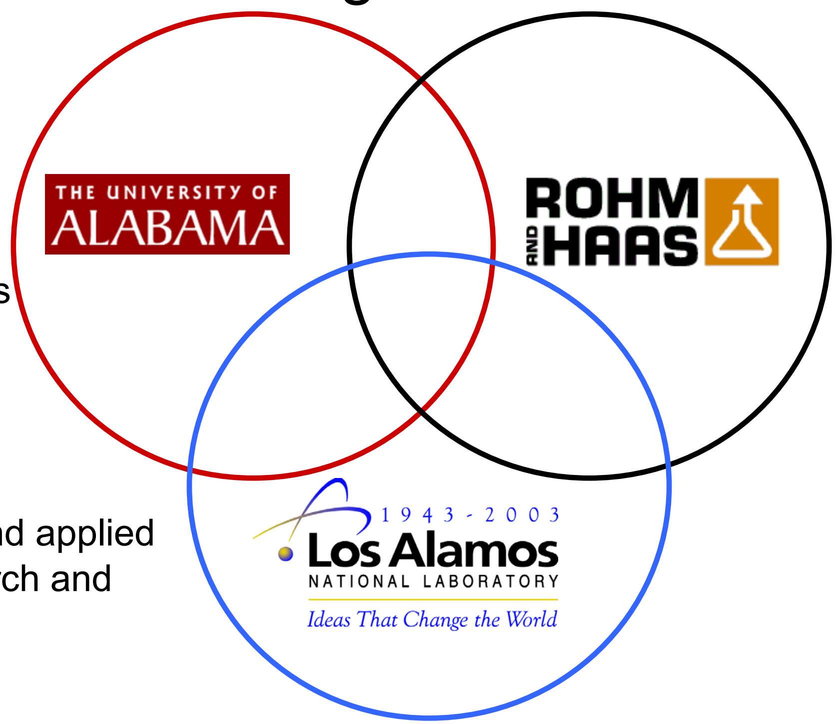
Task 3 – Complexation and Reduction of Borates

- Goal
  - Evaluate various borate complexants for their efficacy in facilitating borate reduction

- Computational thermodynamics
- Fundamental and applied chemical research and development



- Technical archives
- Modeling tools
- Engineering analysis

Task 4 – Electrochemical Reduction of Borates

- Goals
  - Optimize the efficiency of the overall reaction
    $BO_2^- + 6H_2O + 8e^- \rightarrow BH_4^- + 8OH^-$ (aqueous)
  - Validate and optimize previous ROH success with aqueous systems
  - Investigate non-aqueous electrochemical reduction
- Partners
  - LANL, Millennium Cell, Pennsylvania State University

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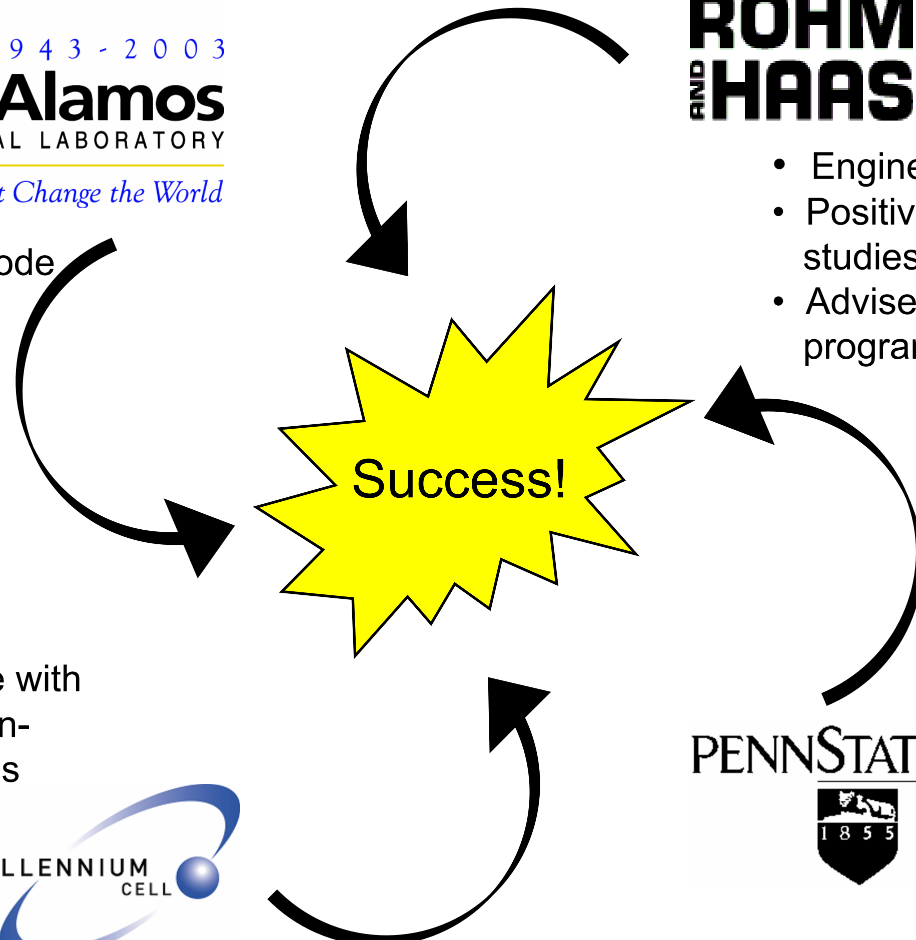
Task 4 – Electrochemical Reduction of Borates



Los Alamos National Laboratory

- Advanced electrode preparation

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- Engineering analysis
- Positive results from past studies (aqueous systems)
- Advise/direct experimental program

Millennium Cell

- Past experience with aqueous and non-aqueous systems

Penn State

- Fundamental insight
- Mechanistic studies
- Advanced analytical development

Accomplishments

- Intellectual Property (IP)
  - Drafted an agreement to cover each participant's rights in IP developed during the project
- Electrochemical Reduction of Borates
  - Kick-off meeting held on March 18, 2005 (LANL, MCEL, PSU, ROH)
  - Established work practices for group
  - Conducted review of prior IP and literature
  - Identified potential experimental studies for aqueous and non-aqueous systems
  - Identified major milestones for Year 1

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Note : This is new project. Start date March 1, 2005

Accomplishments (continued)

- Systems Engineering
  - Kick-off meeting held on March 21, 2005 (PNNL, MCEL, ROH)
  - Established work practices for group
  - Clarified Statement of Work
  - Defined regeneration chemistries
- Hydrogen Safety
  - ROH Safety Plan submitted to DOE on February 24, 2005

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Project Year 1 Milestones

- Finalize IP agreement
- Data Mining / Development of Work Processes
  - Define goals and strategies, boundaries and assumptions; develop performance criteria and metrics
  - Document chemical pathways and process options
- Complexation and Reduction of Borates
  - Establish experimental program
- Electrochemistry
  - Establish appropriate analytical methodology
  - Establish metrics
  - Identify pathways and constraints for B-O to B-H

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Future Work

Task	Year 1 Q1 - 4	Year 2 Q5 - 8	Year 3 Q9 - 12	Year 4 Q13 - 16	Year 5 Q17 - 20
Task 1 Data-Mining	Goals, strategies defined. Performance criteria and metrics developed Chemical pathways and process options documented				
Task 2 Engineering-Guided Research of Chemical Borate Reduction Routes	Leading options for experimental studies identified **(Go/No Go)**	Top option defined **(Go/No Go)**		Top option developed and optimized	Pathway detailed
Task 3 Complexation and Reduction of Borates	Experimental program established Top option defined **(Go/No Go)**			Top option developed and optimized	Pathway detailed
Task 4 Electrochem-ical Reduction of Borates	Establish analytical methodology, metrics. Identify pathways/constraints for B-O to B-H	Top option defined **(Go/No Go)**		Top option developed and optimized	Pathway detailed

Note : Project Start Date March 1, 2005

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