Development of Regenerable, High-Capacity Boron Nitrogen Hydrides For Hydrogen Storage

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Objectives

- Two-Phase, 4-Year, R&D Program to exploit high hydrogen capacity Boron Nitrogen hydrides (Particularly aminoborane, NH_3BH_3) for on-board hydrogen storage
- To develop large-capacity, inexpensive aminoborane synthesis process starting from its decomposition byproduct, boron nitride (BN)
- To develop a simple, efficient, and controllable system for extracting all of the available hydrogen, realizing the high hydrogen density

Technical Targets

- Compact and light-weight hydrogen storage on-board an automobile
- About 5 kg of H_2 need to be stored for > 300 mile range
- DOE's 2015 Targets
  - 0.09 kg H_2/kg of system weight
  - 0.081 kg H_2/L of system volume
  - System cost $67/ kg H_2
  - Fuel cost $1.5/GGE (~kg H_2)

Technical Barriers Addressed

- A – Storage system and fuel cost
- B – Gravimetric/volumetric hydrogen storage density
- C – Energy efficiency
- D – Durability
- E – Refueling Time
- G – System Life-Cycle Assessment
- R – Cost effective regeneration processes
- S – By-Product/Spent Material removal
- T – Thermal Management for hydrogen extraction

Project Timeline

- Project start – March 15, 2005
- Project end – November 30, 2008

Budget

- Total project funding
  - DOE share - $ 1.6M
  - Contractor share - $ 0.4M
- Funding received in FY04 - 0
- Funding for FY05 - $ 0.2M

Collaborating Partners

- State Scientific Research Center of Russian Federation (GNIIChTEOS) - Regeneration of aminoborane starting from its decomposition byproduct, boron nitride (BN)
- ATK/Thiokol – Storage system design and development, Material durability and life-cycle analysis, Technical and economic feasibility analysis

Aminoborane Properties

- Molecular Formula – NH_3BH_3
- White crystalline solid – stable in ambient air
- Hydrogen Content – 19.6% by weight
- Density - 0.74 g/cm3
- Heat of formation - - 42.54 kcal/mole
- Melting temperature ~ 105^{o}C
- Solubility at 20 ^{o}C is ~ 33.6 g in 100 g of water.
- Water solutions of Aminoborane are also very stable during long term storage.

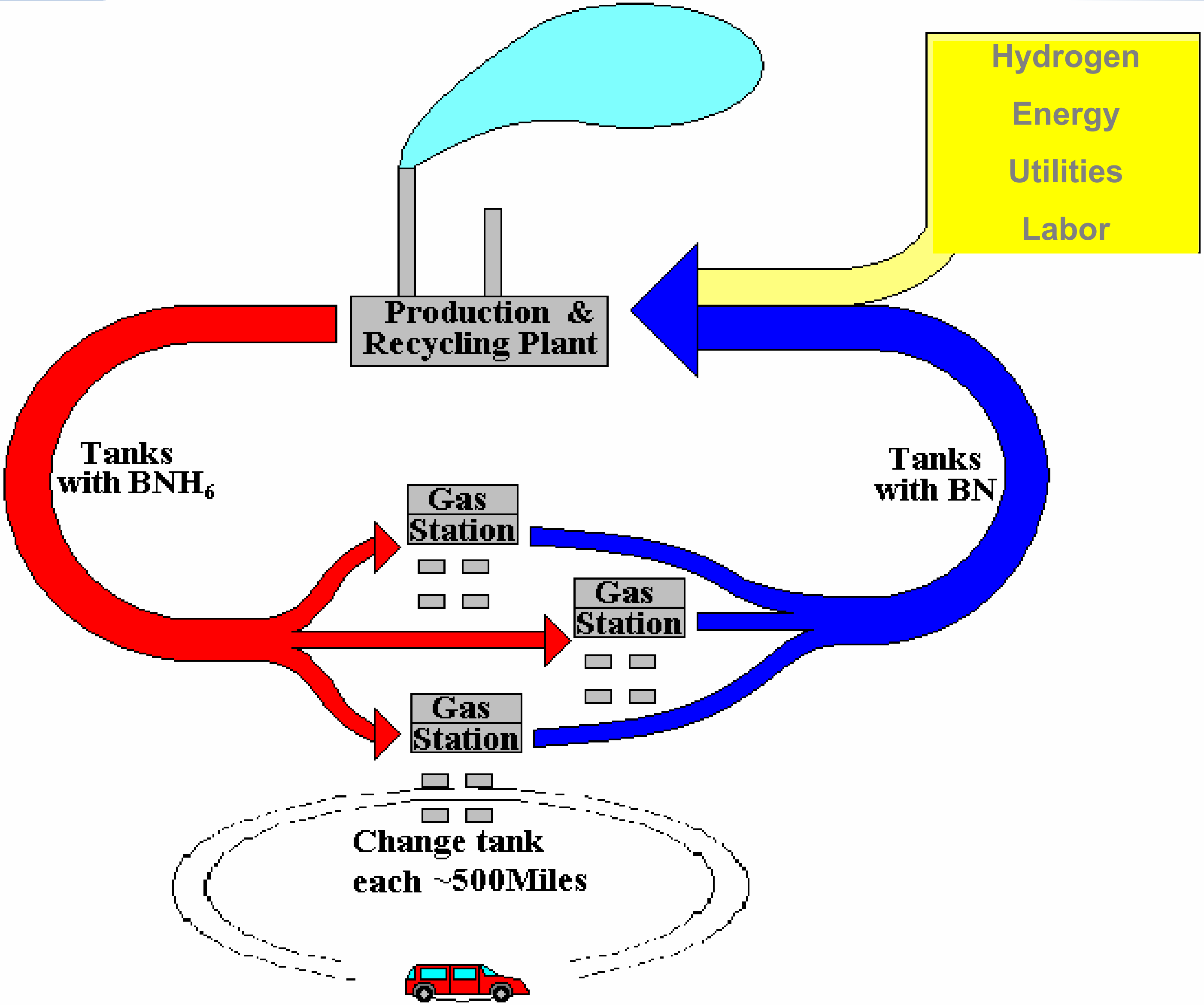
Technical Approach

- Develop large-capacity, inexpensive aminoborane synthesis process starting from its decomposition byproduct, boron nitride (BN) and utilizing commodity hydrogen

- Develop a simple, efficient, and controllable system for on-board heating of aminoborane extracting all of the available hydrogen and realizing a high hydrogen density

Aminoborane for Transportation Application

- On-Demand Decomposition by Direct Heating
- Hydrogen combustion or electrical heating powered by Fuel Cell - Net material-based Hydrogen Density > 17% by wt
- Spent Boron Nitride must be converted to Aminoborane Off-board in a central processing facility utilizing commodity hydrogen
- Develop AB Distribution / BN Recycling Network



Aminoborane in close energy transfer cycle

Specific Program Objectives

- Demonstrate individual steps involved in aminoborane synthesis starting from decomposition (BN) product
- Process integration and scale-up
- Develop on-board hydrogen extraction process
- Design, develop, and demonstrate prototype (1 kg hydrogen capacity) hydrogen extraction system with >9 wt% hydrogen capacity
- Determine technical and economic feasibility

Project Schedule – Phase I (2 Years)

	Tasks	2005										2006												2007	
		M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F
Task 1	Laboratory-scale synthesis of aminoborane (AB) from boron nitride																								
Task 2	Release of Hydrogen from aminoborane																								
Task 3	Feasibility of recycle of AB decomposition products																								
Task 4	Preliminary on-board hydrogen storage system design																		▲						
Task 5	Technical and economic feasibility assessment																								

▲ **Go/No Go Decision**

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Project Schedule – Phase II (2 Years)

	Tasks	2007										2008												2009	
		M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F
Task 6	Scale-up of AB synthesis process using BN and decomposition products																								
Task 7	Integrated process design and development for AB production																								
Task 8	Prototype on-board hydrogen storage system for 1 kg hydrogen																						△		
Task 9	Concept feasibility analysis and Commercialization																								

△ **Deliverable – prototype 1 kg H_2 storage system**

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Activities Planned for FY05

- Task 1 - Laboratory-scale synthesis of aminoborane (AB) from boron nitride – Determination of process conditions and catalysts for maximizing product yield in each of the individual chemical reaction steps
- Task 2 - Release of Hydrogen from aminoborane – Evaluation of heating approaches for maximizing hydrogen yield, thermal modeling of heating system
- Task 4 - Preliminary on-board hydrogen storage system design – Determine requirements of an on-board hydrogen storage and delivery system, preliminary design based on heating approach
- Task 5 - Technical and economic feasibility assessment – Determine costs of stored hydrogen and the storage system using updated information

Activities anticipated in FY06

- Task 1 - Laboratory-scale synthesis of aminoborane (AB) from boron nitride - Finalize process conditions and catalysts for maximizing product yield in each of the individual reaction steps
- Task 2 - Release of Hydrogen from aminoborane – Select a heating approach for maximum hydrogen yield, determine process parameters for hydrogen storage and extraction
- Task 3 - Feasibility of recycle of AB decomposition products – Begin AB synthesis studies using AB decomposition products
- Task 4 - Preliminary on-board hydrogen storage system design – Complete the preliminary design of an on-board hydrogen storage and delivery system using selected heating approach
- Task 5 - Technical and economic feasibility assessment - Update estimates of costs of stored hydrogen and the storage system

Technical Milestones

- Synthesis of pure AB starting from BN at a laboratory scale
- Development, optimization, and demonstration of a process, suitable for on-board deployment, for extraction of pure hydrogen from AB
- Demonstrate lab-scale synthesis of pure AB starting from AB decomposition products
- Design an on-board AB-based hydrogen storage system with > 9 wt% H_2 capacity
- Scale-up AB process to synthesize kg-scale quantities of AB from recycled products
- Development of an integrated process design to convert BN to AB
- Demonstrate a prototype AB based hydrogen storage system to produce 1 kg H_2

Hydrogen Safety

The most significant hydrogen hazards:

- Handling toxic chemicals such as diborane, chlorine, hydrogen and ammonia during evaluation of aminoborane synthesis processes
- Extreme conditions during synthesis processes, e.g. high and low temperatures (e.g. 1000 C to -200 C)
- Uncontrolled release of hydrogen during evaluation of approaches for hydrogen extraction from aminoborane

Hydrogen Safety

Our approach to deal with these hazards:

- Safe laboratory practices during handling of chemicals and extreme process conditions eliminating exposure to TLV levels of toxic chemicals involved.
- Limit scale of experiments to assure safety during synthesis experiments, increasing the scale gradually as experience is gained in handling hazardous process conditions.
- Design hydrogen extraction experiments so as to eliminate any possibilities of uncontrolled release as well exposure of hydrogen to any open flame.
- Conduct all experiments in ventilated fume hood areas