VI.B.5 Development of Regenerable High Capacity Boron Nitrogen Hydrides as Hydrogen Storage Materials

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Objectives

- Demonstrate individual steps involved in aminoborane synthesis starting from pure boron nitride (BN)
- Demonstrate the aminoborane synthesis starting from the aminoborane decomposition product for its recycle
- Scale-up the aminoborane synthesis process
- Develop an integrated process design for aminoborane production
- Evaluate approaches for complete and fast release of hydrogen from aminoborane
- Develop an on-board hydrogen extraction process
- Design an on-board hydrogen storage and extraction system
- Design, develop, and demonstrate prototype (1 kg hydrogen capacity) hydrogen extraction system with >9 wt% hydrogen capacity
- Determine technical and economic feasibility of utilizing aminoborane as an on-board hydrogen storage medium

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- A. Cost

- B. Weight and Volume
- C. Efficiency
- D. Durability
- E. Refueling Time
- R. Regeneration Processes
- S. By-Product/Spent Material Removal
- T. Heat Removal

Technical Targets

This project is evaluating the feasibility of using aminoborane (NH_3BH_3) as an on-board hydrogen storage medium. With 19.6% by weight of hydrogen in its molecular formula, aminoborane has potential to meet DOE's year 2015 targets of gravimetric (0.09 kg H_2/kg of system weight) as well as volumetric (0.081 kg H_2/L of system volume) energy densities. Evaluation of approaches to regenerate aminoborane decomposition products will determine the feasibility of approaching DOE's fuel cost (\$1.5/GGE ~ kg H_2) target. Development of an efficient hydrogen extraction system will allow approaching the storage system cost (\$67/ kg H_2) target.

Approach

The objective of the four-year two-phase project is to develop synthesis and hydrogen extraction processes for nitrogen/boron hydride compounds that will permit exploitation of the high hydrogen content of these materials. The primary compound of interest in this project is aminoborane (NH_3BH_3, ammonia-borane,) a stable white solid at ambient conditions that contain 19.6% of its weight as hydrogen. With a low-pressure on-board storage and an efficient heating system to release hydrogen, aminoborane has a potential to meet DOE's year 2015 specific energy and energy density targets. Amorphous boron nitride (BN) is the desired aminoborane decomposition end-product. If the aminoborane synthesis process could use the BN end-product as the primary starting material, an efficient recycle loop could be set up for converting the BN back into the starting boron-nitrogen hydride.

This project will address two key challenges facing the exploitation of the boron/nitrogen hydrides (aminoborane), as hydrogen storage materials:

- large-capacity inexpensive aminoborane regeneration process starting from its decomposition by-product, BN for recycle, and
- a simple, efficient, and controllable system for extracting all of the available hydrogen, realizing the high hydrogen density on a system weight/volume basis

Phase I will: 1) develop chemical process steps to convert boron nitride to aminoborane, using only hydrogen and commodity chemicals such as ammonia and chlorine, on a laboratory scale, 2) study and optimize the process of hydrogen release by thermal decomposition of aminoborane, 3) demonstrate feasibility of regenerating aminoborane decomposition product, 4) design a preliminary on-board hydrogen storage system and 5) conduct a techno-economic feasibility analysis to provide a go/no go decision for Phase II. With production at a large scale typical of a commodity chemical (as may be expected from a potential gasoline substitute), the cost of aminoborane regeneration has potential to meet DOE's fuel cost targets based on the cost of hydrogen and raw materials used for regeneration. By designing an efficient heating system for aminoborane decomposition, a net high energy density will be realized and the system cost will be minimized approaching DOE's goals.

Upon successful completion of the Phase I, the individual aminoborane synthesis process steps will be integrated and scaled-up in Phase II to be able to synthesize sufficient quantities of aminoborane for testing, demonstration, and delivery to DOE. A prototype on-board hydrogen storage system with 1 kg hydrogen capacity will be designed and fabricated for demonstration of this concept. An integrated process design will be developed for large-scale synthesis of aminoborane and an economic analysis will be conducted to determine the minimum production volume necessary to be able to meet DOE's fuel cost targets.

Accomplishments

- Information available in the literature was reviewed for determining process conditions for chlorination of boron nitride as a first step in its regeneration into aminoborane.
- A high temperature cylindrical furnace/reactor capable of reaching 1,100°C was assembled for studying high temperature boron nitride chlorination.
- Available literature on thermal decomposition of aminoborane was reviewed. The yield of hydrogen and the extent of intermediate product formation strongly depend on the heating profile employed.
- Commercial grade aminoborane was purchased from Fine Boron Compounds, Cleveland, Ohio (A subsidiary of Aviabor) for conducting aminoborane decomposition studies.
- A reactor was designed and fabricated for studying thermal decomposition of aminoborane as a function of operating temperature as well as the residence time at the operating temperature.
- Aminoborane decomposition was studied using thermogravimetric (TGA) as well as differential calorimetry (DSC) techniques in an inert atmosphere. TGA studies indicated aminoborane weight loss substantially greater than that expected from loss of hydrogen alone indicating formation of volatile products during heating.