# Low-Cost $\alpha$-Alane for Hydrogen Storage

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Project ID #
ST116

# Overview

## Timeline

Project Start Date: 15 July 2014
Project End Date: 14 July 2017

Percent complete of activities proposed for FY16: 85%*

* As of 3/26/16

## Barriers

- Low-cost production of $\alpha$-alane by electrochemical / chemical pathways
- Engineering cost analysis of entire alane synthesis and regeneration process
- Conservation of lithium aluminum hydride electrolyte
- Development of a particle bed reactor

## Budget

Total Project Budget: $1,500,514

- Total Recipient Share: $301,266
- Total Federal Share: $1,199,248
- Total DOE Funds Spent*: $722,566

## Collaborators

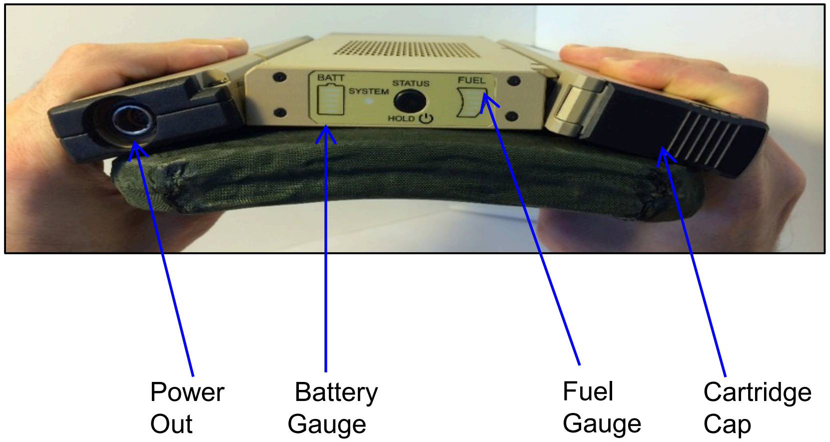
- SRI International (Subcontractor)
- SRNL (CRADA Partner)

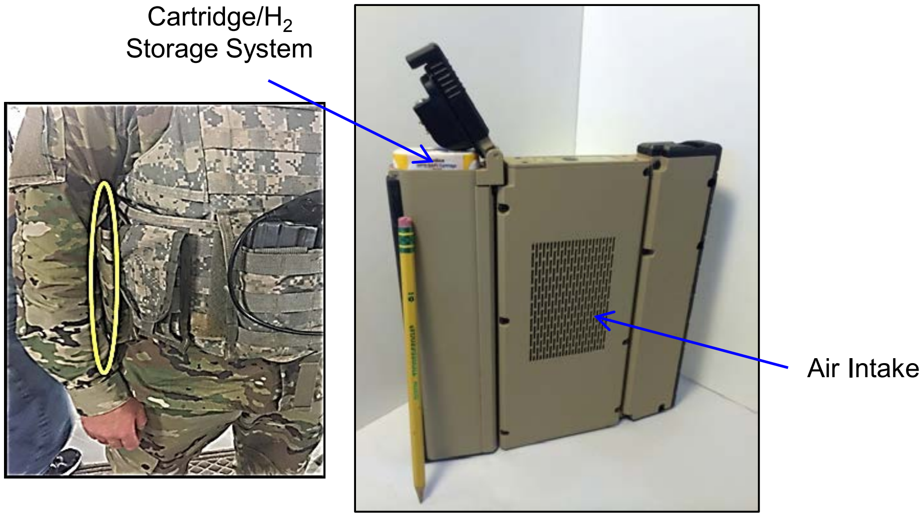
# Relevance: Project Objectives

**Overall**: Reduce production cost of $\alpha$-alane ($AlH_3$) to meet the DOE 2015 and 2020 hydrogen storage system cost targets for portable low- and medium-power applications. Enables broader applications in consumer electronics (smart phones, tablets, laptops…), back-up power, UAVs, forklifts, and vehicles.

- Perform engineering cost analyses of electrochemical and chemical processes to meet the cost targets for synthesis and regeneration of $\alpha$-alane throughout the program
- Demonstrate practical *electrochemical process* to synthesize alane adduct building on SRNL's pioneering work that can be transitioned to a large-scale facility
- Develop an electrochemical particle bed design approach that enables increased rate of reaction and a (semi-) continuous process
- Demonstrate recovery of $MAlH_4$ (M = Li, Na) electrolyte
- Develop an efficient process for recrystallization, passivation and formulation of the alane product

# Relevance: Wearable Power System for a Dismounted Soldier (WPS20)*





*One example of a high-value application

| Features | |
|---|---|
| Fuel | $\alpha$-alane (85 grams per cartridge) |
| Dimensions | 7” x 8” x 0.89” with flexibility to conform to a small arms protective insert (SAPI) plate |
| Power Output | 20 W continuous, 35 W peak |
| Cartridge/$H_2$ Storage System Energy Density | 1.03 KWh/kg, 1.32 KWh/L (72h at 20W continuous) |
| System Compatibility | Standards for soldier power distribution manager |

# Approach: Aluminum Particle Bed Reactor

**Background**

(**R1**) $3\ LiAlH_4 + Al_{metal} \rightarrow 4\ AlH_3 + 3\ Li^+ + 3\ e^-$

(**R2**) $LiAlH_4 \rightarrow AlH_3 + 1/2H_2 + Li^+ + e^-$

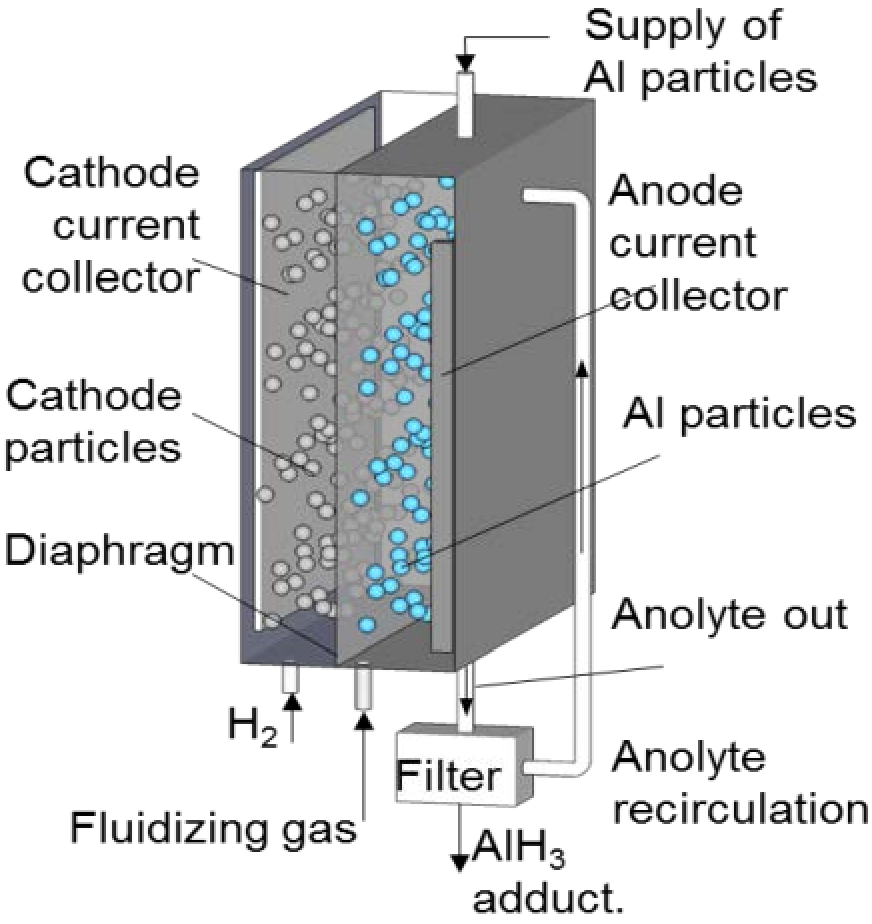
(Anode reactions)

- Electrochemical process developed by SRNL
- Uses $NaAlH_4$ or $LiAlH_4$ electrolyte and Al anode

**Proposed Particle Bed Reactor**

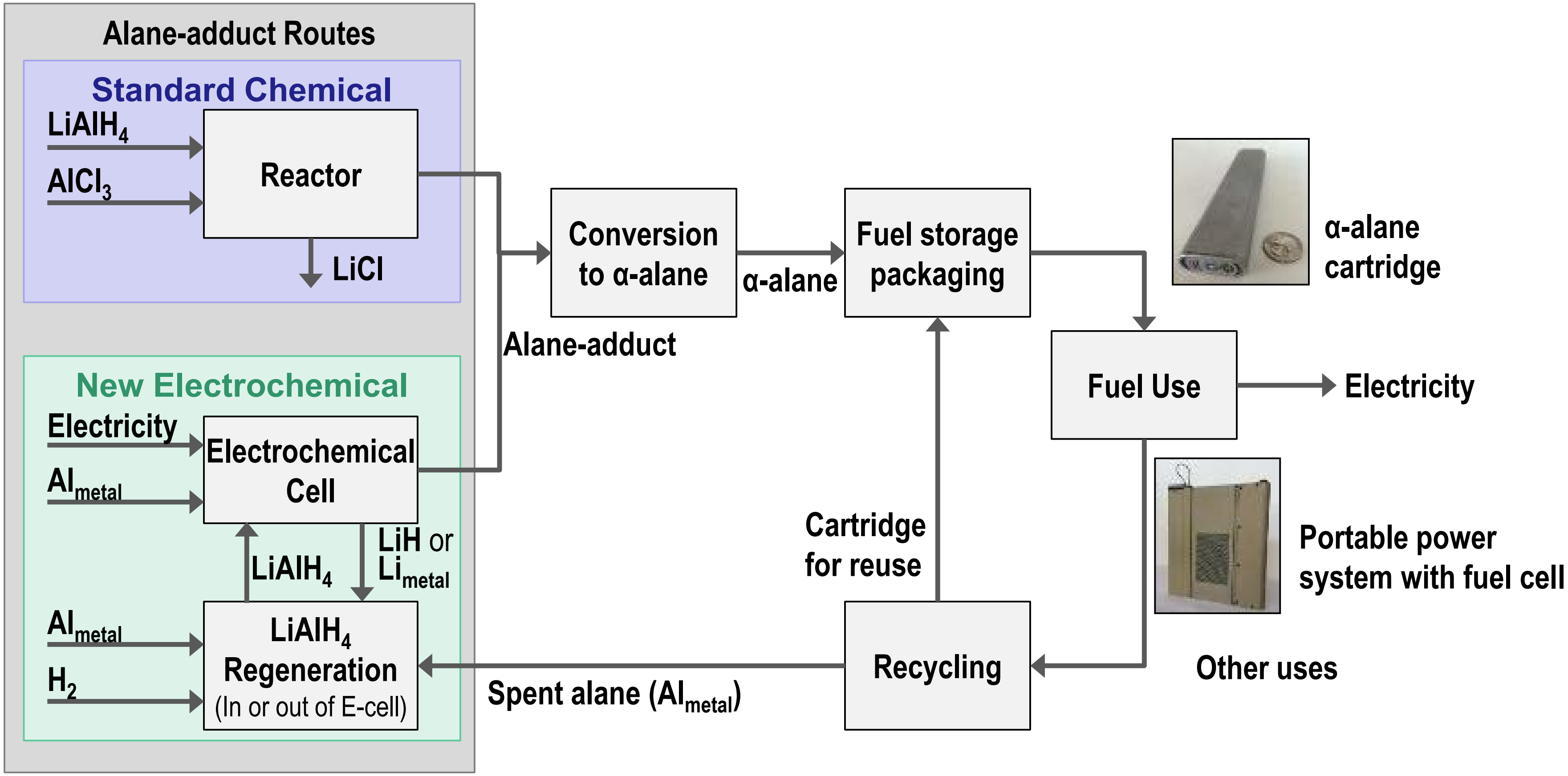
- Bed of conductive particles act as electrodes, ideally both anode and cathode
- High surface to volume enhances kinetics, enabling high current and throughput. Potential for continuous process.
- Regeneration of $LiAlH_4$ now feasible

**Schematic illustration of dual-particle bed reactor**



# Approach: Electrolysis Process added to Alane Production

Reducing costs in the chemical process is difficult due to feedstock costs. Changing the front end to the electrolysis process for alane adduct production can reduce these costs.



**Alane-adduct Routes**

**Standard Chemical**

$LiAlH_4$

$AlCl_3$

Reactor

LiCl

**New Electrochemical**

Electricity

$Al_{metal}$

Electrochemical Cell

$LiAlH_4$

LiH or $Li_{metal}$

$Al_{metal}$

$H_2$

$LiAlH_4$ Regeneration (In or out of E-cell)

Alane-adduct

Conversion to α-alane

α-alane

Fuel storage packaging

α-alane cartridge

Fuel Use

Electricity

Portable power system with fuel cell

Other uses

Cartridge for reuse

Recycling

Spent alane ($Al_{metal}$)

# Approach: Process and Economic Modeling Methodology

## Process Modeling:

- Process flow diagram and mass/energy balance for all unit operations.
- End-to-end process including feedstock preparation, down-stream chemical workup, and materials recycling and regeneration.

## Economic Modeling:

- Using methodology laid out by Peters, Timmerhaus, and West[1]
- Higher multipliers and ratio factors account for increased costs associated with the safety and air sensitive materials handling requirements of this process compared to a typical chemical process.

## Work Flow

**Process Flow Diagram**
- Identify all process steps and unit operations for the end-to-end synthesis→ process flow diagram

**Mass & Energy Balance**
- Perform a mass and energy balance across all unit operations → estimate materials and utilities

**Equip. Sizing**
- Identify equipment, materials of construction, and estimate hold-up/residence times

**Capital Equip. Costs**
- Utilize tables & formulas, with multipliers for materials/features → estimate capital equipment costs

**Total Capital**
- Estimate total capital costs from the capital equipment costs using ratio factors

**Labor**
- Estimate labor requirement via number of staff per shift and wages

**Other Costs**
- Estimate other production costs, fixed expenses, and general expenses using ratio factors

**Alane Product Cost**

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[1] Peters, M. S., Timmerhaus, K. D., West, R. E., Plant Design and Economics for Chemical Engineers, Fifth Edition, McGraw Hill (2003).

# Approach: Cost Reduction Compared to the Chemical Synthesis Route to Alane

Electrochemical process reduces alane cost from an improved, consumable aluminum anode to regenerate $LiAlH_4$ and optimize recycling of unreacted $LiAlH_4$.

| Storage System Costs | | | Current Cost | Chemical Route (1,2) | Electrochemical Route | | |
|---|---|---|---|---|---|---|---|
| | | | | | Baseline (1,3) | Cathode Recycle (1) | Increased Scale to 3,200 MT/yr |
| | | | Pilot Plant | Commercial Scale | (80% AlH3 from R1) | (80% AlH3 from R1, 80% LiAlH4 regenerated) | (80% AlH3 from R1, 80% LiAlH4 regenerated) |
| Alane Fuel Costs | | $/kg alane | 3500 | 112 | 81 | 56 | 29 |
| Cartridge Cost (4) | | $/kg alane | 79 | 53 | 53 | 53 | 44 |
| Total | | $/kg alane | 3579 | 165 | 134 | 109 | 73 |
| Storage System Cost | | $/g H2 | 38.91 | 1.79 | 1.46 | 1.18 | 0.79 |
| **DOE Metrics** | | **$/g H2** | | **Target Met?** | | | |
| Low Power | 2015 | 3 | N | Y | Y | Y | Y |
| | 2020 | 1 | N | N | N | N | Y |
| Medium Power | 2015 | 6.7 | N | Y | Y | Y | Y |
| | 2020 | 3.3 | N | N | N | Y | Y |

Production cost broken down in later slides

1. Chemical and electrochemical route productions costs are for a 320 MT/yr process.
2. Commercial scale estimate provided by Albemarle.
3. Cost of alane entirely from reaction (R2) is $101, compared to $81 for 80% from reaction (R1).
4. New cartridge costs based on manufacturer estimates. $79/kg $AlH_3$ at small scale production, $53/kg $AlH_3$ at 4 M cartridges/year and $44//kg $AlH_3$ at 20 M cartridges/year. Further cost savings of 25-33% per cartridge can be realized through recycling, not shown.

## Baseline (Anode Reactions)

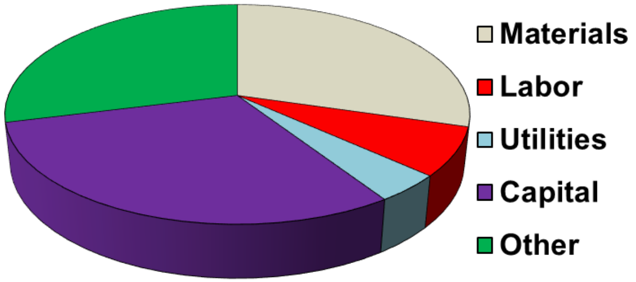
(**R1-80%**) $3\ LiAlH_4 + Al_{metal} \rightarrow 4\ AlH_3 + 3\ Li^+ + 3\ e^-$

(**R2-20%**) $LiAlH_4 \rightarrow AlH_3 + 1/2H_2 + Li^+ + e^-$

# Approach: Process and Economic Modeling

Detailed economic model example shows alane production cost of $56 per kg from the electrochemical process in which $\alpha$-alane is produced from an aluminum anode via an N-ethylmorpholine adduct and $LiAlH_4$ is regenerated from the cathode by-products.

| Production Costs | Basis | $/kg |
|---|---|---|
| Raw materials | Mass balance | $ 16 |
| Labor | Labor estimate | $ 4 |
| Utilities | Energy balance | $ 2 |
| Capital costs (depreciation and financing) | Capital Estimate | $ 17 |
| Other (Maintenance, supplies, plant and admin overhead, etc.) | Various ratio factors | $ 16 |
| **Total Product Cost** | | **$ 56** |



**Key Assumptions:**

- 320 MT/yr
- 80% $AlH_3$ is from R1
- 5 V cell potential, incl. ohmic losses
- Current density is 150 mA/cm$^2$
- $LiAlH_4$ is recovered from cathode by-products with an 80% yield
- N-ethylmorpholine (NEM) adduct is employed
- $LiAlH_4$ is made from $NaAlH_4$ ($NaAlH_4$ supplier cost $20/kg)
- Fully recover and recycle the solvents, NEM, and $LiAlH_4$ that persist into downstream processes

Sensitivity Analysis: Largest cost savings from starting material cost and scale of production

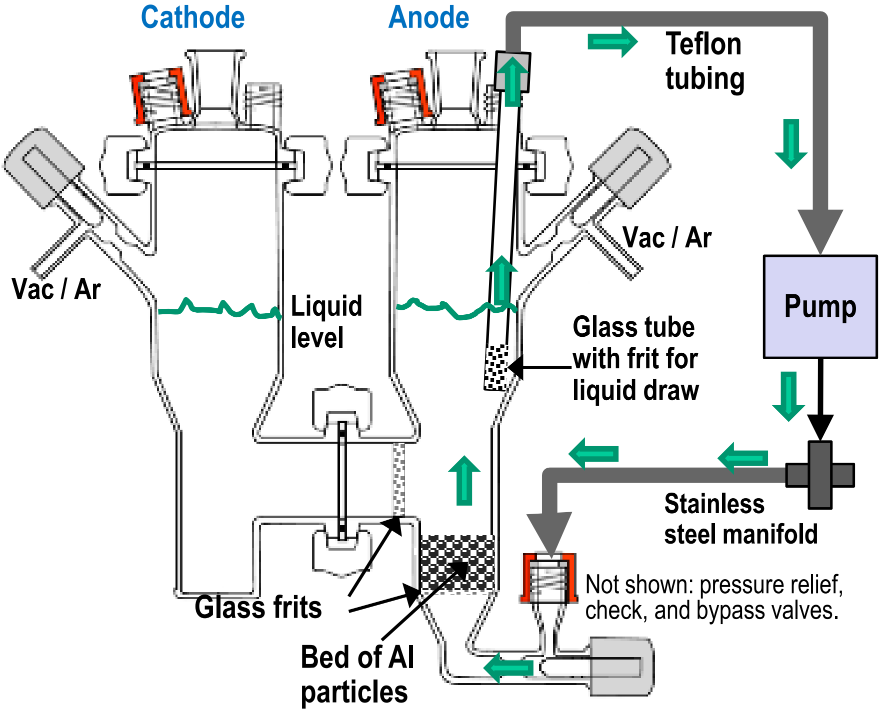
| $NaAlH_4$ Cost ($/kg) | Product Cost ($/kg $AlH_3$) |
|---|---|
| 100 | 102 |
| 20 | 56 |
| 5 | 47 |

| Potential (V) | Cell Electrical Cost ($/kg $AlH_3$) | Product Cost ($/kg $AlH_3$) |
|---|---|---|
| 3 | 0.23 | 56 |
| 5 | 0.38 | 56 |
| 10 | 0.77 | 56 |

| Annual Production (MT/yr) | Capital Investment ($M) | Product Cost ($/kg $AlH_3$) |
|---|---|---|
| 320 | 36 | 56 |
| 3,200 | 120 | 29 |
| 32,000 | 720 | 23 |

# Technical Accomplishments: Particle Bed Fabrication & Operation

- SRI and Prof. Jim Evans (UC Berkeley) settled on a simple particle bed design that utilizes an anode compartment composed of aluminum particles over a porous glass frit fluidized to a variable degree by a reversible and variable flow of electrolyte
- Simple design facilitates rapid assembly and cleanup
- Allows evaluation of different aluminum particles sizes
- Facilitates the evaluation of electrolyte flow rate and flow direction to optimized fluidization vs particle size



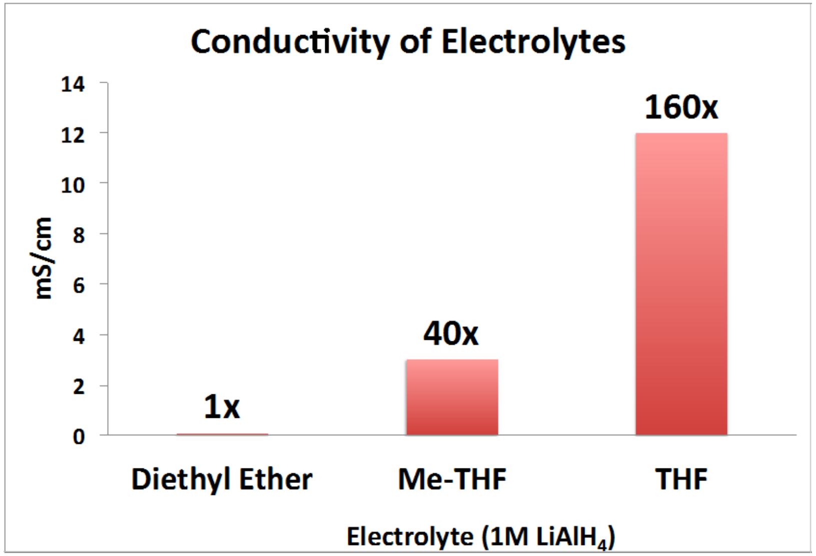
Not shown: pressure relief, check, and bypass valves.

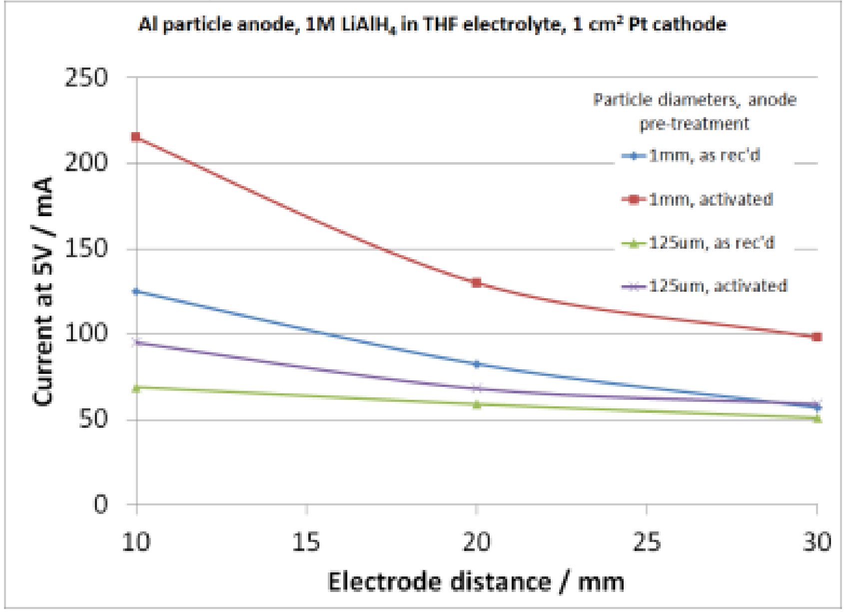
# Technical Accomplishments: Understanding Aspects of Cell Design and Operation

*Design critical for optimized cell conductance*

Choice of electrolytic solvent:

- THF-based electrolytes provide strikingly higher conductivities compared to diethyl ether.
- Conductivity increase linearly with $LiAlH_4$ concentration.
- Electrolyte additives LiX (X = Cl, Br and I), N-ethylmorpholine and glymes to 1M $LiAlH_4$ in diethyl ether or THF have no significant effect on conductivity.





- As expected, reduction of electrode spacing increases current dramatically.
- Activation of Al particles with 10% aqueous NaOH removes oxides. Up to 70% current increase observed.
- Smaller particles give lower current likely due to higher oxide content. Improve with better activation techniques.

# Scaling the Electrochemical Vision

**Assumptions:**

- For a 320,000 kg/yr (292 days/yr) plant:

  → 46 kg/h (1.6 kmol/h) $AlH_3$

- Assume 80% of alane is produced from R1:

  → ~33 kA of current required

- Cell contains 1 $m^2$ of consumable anode area

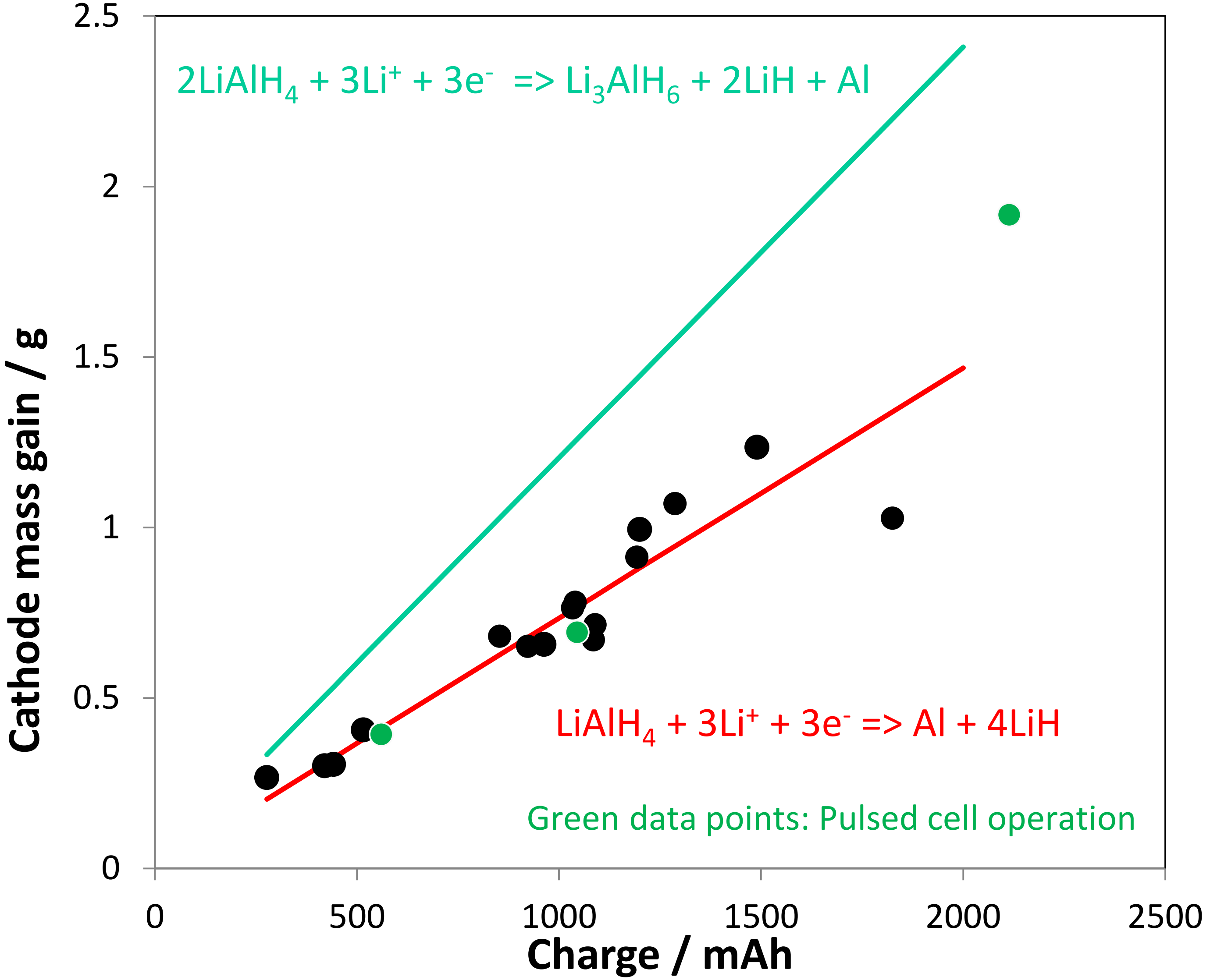
**Key design considerations**

- Balance needs for minimal (solvent) volume and thermal management;
  - → Recirculating electrolyte
- Minimal electrode spacing for high current density
- Optimized current pulse protocol
  - → Avoid cathode dendrite formation
  - → Maintain practical net anodic current density
  - → Facilitate cathode product collection

| Current Density ($mA/cm^2$) | Number of Cells | Alane Production Rate* (kg/h) / cell | Adduct Production Rate** (kg/h) / cell | $LiAlH_4$ Consumption Rate (kg/h) / cell | Power Dissipation @ 5V applied*** kW / cell |
|---|---|---|---|---|---|
| 50 | 66 | 0.7 | 2.4 | 1.0 | 2.2 |
| 100 | 33 | 1.4 | 4.8 | 1.9 | 4.3 |
| 200 | 17 | 2.8 | 9.6 | 3.8 | 8.6 |

* Alane content of adduct; ** $AlH_3 \cdot THF$ adduct; *** OCV: 0.7 V

# Technical Accomplishments: Cathode Reaction Products are Predominantly Al and LiH



*Pulsed cell parameters based on SRNL work

# Technical Accomplishments: Cathodic Processes

Cathode product composition is sensitive to electrolytic solvent, electrode distance and electrochemical cell operational parameters.

$LiAlH_4$ may be consumed in various cathode-related reactions:

A. $2LiAlH_4 + 3Li^+ + 3e^- \rightarrow Al + 2LiH + Li_3AlH_6$

B. $LiAlH_4 + 3Li^+ + 3e^- \rightarrow Al + 4LiH$

- Diethyl ether based electrolytes give $Li_3AlH_6$ complex and Al. Tetrahydrofuran based electrolytes give a mixture of 4LiH and Al (by XRD, IR and Elemental Analysis). We hypothesize that this difference is due to the in-situ conversion of $Li_3AlH_6$ in more polar solvents.[1] $3Li_3AlH_6 \rightarrow Al + 2LiH + LiAlH_4$
- Reverse pulse method deposits identical mass of cathode materials in a laminar configuration that allows reduction in inter-electrode distances. Traps $Li_3AlH_6$.

Enables regeneration of electrolyte $MAlH_4$ from captured cathodic materials ($Li_3AlH_6$, LiH and Al)[1]

C. $Li_3AlH_6 + 2Al + 3H_2 \rightarrow 3LiAlH_4$

D. $2LiH + 2Al + 3H_2 \rightarrow 2LiAlH_4$

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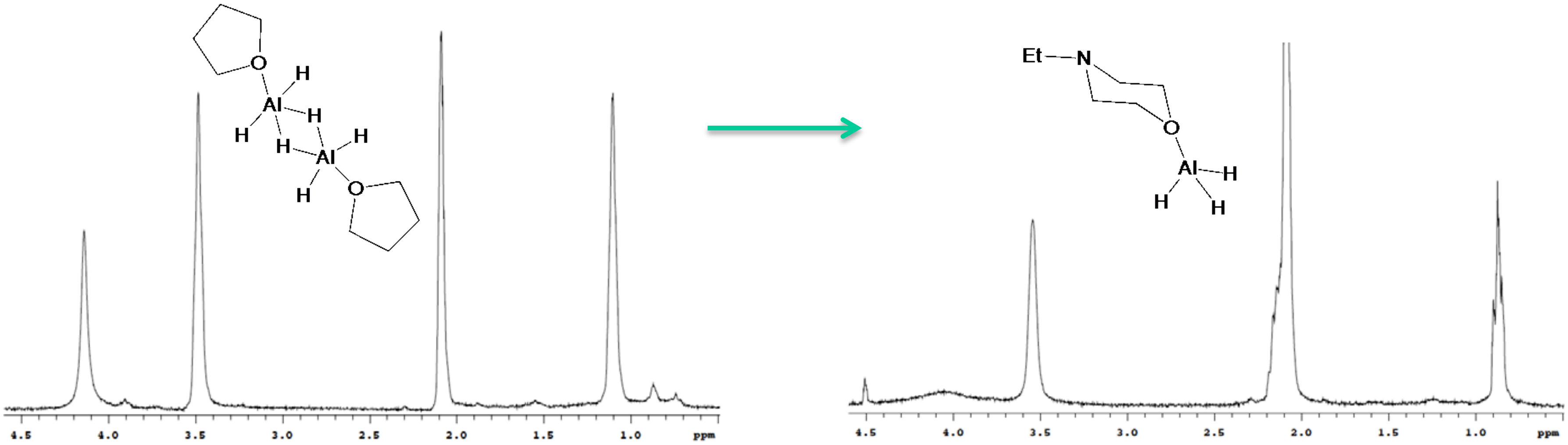
1) **Murib, J. H. U.S. Patent 3,649,223, March 4, 1972; Beaird Jr., F. M.; Kobetz, P. U.S. Patent 3,355,262, November 28, 1967.**

# Technical Accomplishments: Successful separation of a useful alane adduct from $NaAlH_4$/THF based electrolyte.

Verified by $^1$H NMR and XRD[1]



**Alane THF adduct dimer is isolated then converted to the N-ethylmorpholine adduct**

We can isolate an adduct from a highly conducting electrolyte (e.g. $NaAlH_4$/THF) that can reportedly be converted into $\alpha$–$AlH_3$. $NaAlH_4$/THF based electrolyte facilitates isolation of the N-ethylmorpholine (NEM) adduct due to lower energy of solvation ($Na^+$ vs. $Li^+$). Conversion to $\alpha$–$AlH_3$ currently being optimized.

J. Graetz et al reported N-ethylmorpholine adduct can be converted to $\alpha$-$AlH_3$[1]

1) Chengbao, N.; Yang, L.; Muckerman, J. T.; and Graetz, J. , *J. Phys. Chem. C* **2013**, *117*, 14983-14991

# Collaborations

| **Collaborators** | **Role** |
|---|---|
| **Ardica Technologies**: Dick Martin (PI)<br>(Receiving DoE project funds) | Development of alane-based hydrogen storage system for portable power |
| **SRI International**: Mark Petrie (PI), Steve Crouch-Baker, David Stout, Fran Tanzella<br>(Receiving DoE project funds) | Development of low-cost electrochemical and chemical synthesis production methods for alane production scale-up |
| **SRNL**: Ragaiy Zidan<br>(Receiving DoE funds through a related project) | Development of novel methods for the synthesis of low-cost alane |
| **Albemarle:** John Parks<br>(Receiving Ardica funds) | Industrial partner for the scale up of alane production. Currently optimizing the chemical route. |
| **UC Berkeley:** Prof. James Evans<br>(Receiving Ardica funds) | Expert advisor on fluidized bed design |

# Remaining Challenges and Barriers

- Minimize cell resistance through cell design; construction, testing of a scalable cell design to increase the rate of alane production

- Regeneration of $LiAlH_4$ from the products generated on the cathodic side of the cell

- Facile isolation of a stable alane adduct from the electrochemical reaction that is readily converted to alpha alane (e.g. N-ethylmorpholine or triethylamine alane adduct)

# Proposed Future Work

1. Design, fabricate, and test a scalable particle bed cell that builds on our experience with the H-cell that optimizes electrode kinetics, enables high-current, and hence high-throughput operation. Collaboration with Prof. Evans (UCB) is critical for this activity. (2016-2017)

2. Deposition of cathode products at high activity and yield for further reaction and regeneration of lithium or sodium aluminum hydride ($MAlH_4$). Modify pulse methods and fluidization of cathodic bed aluminum particles for deposition/capture of these materials. Improve morphology and optimize conversion to $MAlH_4$ (2016-2017)

3. Optimize solvent swap methods for complete separation of alane adduct from the concentrated $NaAlH_4$ based electrolyte. Optimize thermal conversion to $\alpha$-alane from amine adducts using crystallization aides and heating profiles. (2016-2017)

# Project Summary

## Evaluate electrochemical/chemical routes to reduce alane synthesis cost

- Full engineering cost analysis of electrochemical and chemical processes to meet DOE metrics
- Initial analysis shows the electrochemical synthesis affords a max. ~50% reduction in alane cost

## Maximize electrolyte ($LiAlH_4$) recovery in electrochemical alane synthesis

- Characterized and modified morphology of materials deposited ($Li_3AlH_6$ + LiH + $Al_{(metal)}$) on the cathodic side of the cell
- Strategies include electrolytic solvent, electrode distance and electrochemical cell operational parameters

## Optimize particle bed EC reactor (moving or static)

- Designed, constructed and characterized particle bed reactor
- Evaluated reactor as a function of particle size and flow rates
- Continued collaboration with Prof. James Evans for particle bed design

## Separation of alane from the concentrated electrolyte

- Partially recovered alane produced in an electrochemical cell using a THF/$NaAlH_4$ electrolyte.
- Need to optimize transformation of the alane adduct to the alpha alane product

# Technical Back-Up Slides

# Model Details –
# Estimated Materials Requirements

- Estimated from an Excel based mass balance for all steps shown in the flow diagram.
- The quantities are automatically adjusted as the model variables are changed including: total annual production quantity of alane; reaction yields; concentrations; and extents of recycling, recovery, or separation.
- Bulk chemical prices were sourced from chemical manufacturing companies.

| Material | Cost | | Source | Amounts | | | Costs | |
|---|---|---|---|---|---|---|---|---|
| | $/kg | | | kg/hr | kg/yr | kg/kg AlH3 | $/yr | $/kg AlH3 |
| **Reactants & Consumables** | | | | | | | | |
| Hydrogen gas | $ | 2.00 | Cost target from EERE report | 4.39 | 30,741 | 0.10 | 61,482 | 0.19 |
| Aluminum | $ | 1.81 | Vincent Metals | 43.17 | 302,521 | 0.95 | 547,564 | 1.71 |
| Sodium aluminum hydride | $ | 20.00 | Albemarle | 26.56 | 186,101 | 0.58 | 3,722,013 | 11.65 |
| Lithium chloride | $ | 5.00 | Albemarle | 20.85 | 146,103 | 0.46 | 730,514 | 2.29 |
| Hydrochloric acid | $ | 0.26 | Shijiazuang Xinlonwei | 9.78 | 68,503 | 0.21 | 17,811 | 0.06 |
| | | | | | | **Total** | **5,079,384** | **15.89** |

Notes:

| | | |
|---|---|---|
| Assumed Operational time | 292 | days/yr |
| Hourly AlH3 production rate | 45.6 | kg/hr |
| Annual AlH3 production rate | 319,622 | kg/yr |

Hydrogen cost based on anticipated production cost from EERE report

# Model Details – Estimated Utilities Requirements

- Estimated from an Excel based energy balance for all steps shown in the flow diagram.
- The heating and cooling requirements are determined by the heat capacities, heat of reactions, and heat of vaporization; all of which are included in the model. The pumping requirements are estimated based on hourly volumetric throughput of the system.
- The other power requirements are only a rough estimate due to the lack of specific equipment detail at this point, however this quantity is almost negligible compared to the other energy requirements.

| Unit Operation Name | Power Req'ts MJ/hr | Annual Energy Req'ts kWhr | Annual Energy Cost $/yr | Cost per kg Alane $/kg $AlH_3$ |
|---|---|---|---|---|
| **Electrochemistry** | | | | |
| **Electrochemical cell** | **617** | **1,201,738** | **$ 122,457** | **$ 0.383** |
| **Heating** | | | | |
| Alane etherate concentration | 465 | 906,133 | | |
| Alane etherate flash | - | - | | |
| Solvent swap evaporation | 102 | 197,843 | | |
| Heating for crystallization | 61 | 118,807 | | |
| Solvent distillation reboiler | 476 | 927,458 | | |
| Wet solvent distillation reboiler | 257 | 499,698 | | |
| Ether removal, $LiAlH_4$ regeneration | 19 | 36,724 | | |
| Solvent removal, $LiAlH_4$ regeneration | 132 | 257,552 | | |
| **Heating Total** | **1,512** | **2,944,215** | | |
| **Total with heat integration/recovery** | **1,512** | **2,944,215** | **$ 300,016** | **$ 0.939** |
| **Cooling** | | | | |
| Alane etherate concentrate condenser | 465 | 906,133 | | |
| Alane etherate flash condenser | - | - | | |
| Solvent swap condenser | 102 | 197,843 | | |
| Crystallization condenser | 11 | 21,837 | | |
| Post crystallizaiton cooling | 63 | 122,300 | | |
| Solvent distillation, ether condenser | 10 | 20,182 | | |
| Solvent distillation, toluene condenser | 385 | 749,298 | | |
| Alane dryer condenser | 41 | 79,190 | | |
| Wet solvent distill, ether condenser | - | - | | |
| Wet solvent distill, toluene condenser | 257 | 499,698 | | |
| Solids neutralization | 0.01 | 27 | | |
| Ether condenser, $LiAlH_4$ regen. ether removal | 18.86 | 36,724 | | |
| Solvent condenser, $LiAlH_4$ regen. solvent removal | 5.49 | 10,694 | | |
| **Cooling Total** | **1,358** | **2,643,926** | | |
| **Total with heat integration/recovery** | **1,358** | **2,643,926** | **$ 269,416** | **$ 0.843** |
| **Pumping (liquid and vacuum)** | | | | |
| Estimate of total pumping | **80** | **155,733** | **$ 15,869** | **$ 0.050** |
| **Other** | | | | |
| Est. of controls, instruments, agitation, heat integration, etc. | **100** | **194,667** | **$ 19,837** | **$ 0.062** |
| **Total energy costs** | | | **$ 727,594** | **$ 2.276** |

**Notes:**

| | | |
|---|---|---|
| Assumed Operational time | 292 | days/yr |
| Hourly $AlH_3$ production rate | 45.6 | kg/hr |
| Annual $AlH_3$ production rate | 319,622 | kg/yr |
| Electricity cost | 0.1019 | $/kWhr |

# Model Details – Estimated Capital Investment

- Capital equipment sizes are based on the estimated throughput from the mass balance for all process steps shown in the flow diagram
- Purchase costs were determined primarily from literature table cost estimates along with some from vendor estimates. Multipliers were used to adjust the cost for materials of construction and the handling of air sensitive materials.
- The total delivered capital equipment cost is used to determine the total capital cost using ratio factors following the method first proposed by Lang[1,2]. We used values reported in Peters, Timmerhaus, & West for fluid processing plants.
- Due to the air sensitive materials handling and safety requirements, we used factors for installation, piping, and building costs that were at the higher end of the ranges for chemical plants.

| | Approximate Ranges* | Value (%) | Cost ($) |
|---|---|---|---|
| **Direct Costs** | | | |
| Purchased equipment delivered | | | 4,806,978 |
| Purchased equipment installation | 25-55% of purchased | 55 | 2,643,838 |
| Instrumentation and controls (installed) | 6-30% of purchased | 25 | 1,201,745 |
| Piping (installed) | 10-80% of purchased | 80 | 3,845,582 |
| Electrical (installed) | 10-40% of purchased | 20 | 961,396 |
| Buildings (including services) | 10-70% of purchased | 70 | 3,364,885 |
| Yard improvements & service facilities | 40-100% of | 80 | 3,845,582 |
| Land | 4-8% of purchased | 4 | 192,279 |
| **Total Direct Costs** | | | **$ 20,862,285** |
| **Indirect** | | | |
| Engineering and supervision | 5-30% of direct costs | 15 | 3,129,343 |
| Construction expenses and contractor's fee | 6-30% of direct costs | 25 | 5,215,571 |
| Contingency | 5-15% of fixed-capital | 10 | 3,245,244 |
| **Total Indirect Costs** | | | **$ 11,590,158** |
| **Fixed Capital Investment** | | | **$ 32,452,443** |
| Working Capital (15%) | 10-20% of total capita | 10 | 3,605,827 |
| **Total Capital Investment** | | | **$ 36,058,270** |

* Ranges from Peters & Timmerhaus for fluid processing.

Annual $AlH_3$ production rate 319,622 kg/yr

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1) Lang., H. J., Cost relationships in preliminary cost estimation, Chem. Eng., 54(10):117 (1947).

2) Lang., H. J., Simplified approach to preliminary estimates, Chem. Eng., 55(6):112 (1948).

# Model Details -
# Estimated Manufacturing Cost

- The total production cost uses methodology described in Peters, Timmerhaus, and West which provides ranges that are typical for chemical processes.
- In our model, the baseline values for the additional estimates are chosen to be the middle of the ranges; however these are easily adjusted in the model.
- The alane process varies from the approximate ranges in regards to a high raw materials cost (depending on what variables are selected).
- Currently the 'patents and royalties' cost is to be determined, while the 'distribution and selling' and 'research and development' costs are ignored.

| | Approximate Ranges (Peters, Timmerhaus, & West) | Value Used | Basis | $/yr | $/kg |
|---|---|---|---|---|---|
| **Manufacturing Costs** | | | | | |
| **Direct Production Costs** | | | | | |
| Raw Materials | (10-50% of total product cost) | Materials table | Mass balance | $ 5,261,015 | $ 16.46 |
| Operating Labor | (10-20% of total product cost) | Labor Table | Labor est. | $ 946,080 | $ 2.96 |
| Supervisory and Clerical Labor | (10-25% of operating labor) | Labor Table | Labor est. | $ 322,368 | $ 1.01 |
| Utilities | (10-20% of total product cost) | Energy Table | Energy balance | $ 727,594 | $ 2.28 |
| Maintenance and Repairs | (2-10% of fixed-capital investment) | 5% | RF of fixed capital | $ 1,622,622 | $ 5.08 |
| Operating Supplies | (10-20% of maintenance and repairs) | 15% | RF of maint. & rep. | $ 243,393 | $ 0.76 |
| Laboratory Charges | (10-20% of operating labor) | 15% | RF of operating labor | $ 141,912 | $ 0.44 |
| Patents & Royalties | (0-6% of total product costs) | TBD | | $ - | $ - |
| **Total Direct Costs** | | | | **$ 9,264,985** | **$ 28.99** |
| **Fixed Charges** | | | | | |
| Depreciation (Capital Costs) | (10% of fixed capital, 2-3% of building) | 10% | Capital Estimate | $ 3,605,827 | $ 11.28 |
| Local Taxes | (1-4% of fixed capital) | 2% | RF of fixed capital | $ 649,049 | $ 2.03 |
| Insurance | (0.4-1% of fixed capital) | 1% | RF of fixed capital | $ 324,524 | $ 1.02 |
| **Total Fixed Charges** | | | | **$ 4,579,400** | **$ 14.33** |
| **Plant Overhead costs** | (50-70% of total labor & maint. costs) | 60% | RF of labor & maint. | **$ 1,734,642** | **$ 5.43** |
| **Total Manufacturing Cost** | Sum of direct, fixed, and plant overhead. | | | **$ 15,579,027** | **$ 48.74** |
| **General Expenses** | | | | | |
| Administrative | (15% of total labor & maint. costs) | 15% | RF of labor & maint. | $ 433,661 | $ 1.36 |
| Distribution and Selling | (2-20% of total product cost) | 0% | | $ - | $ - |
| Research and Development | (2-5% of total product cost) | 0% | | $ - | $ - |
| Financing | (0-10% of total capital investment) | 5% | RF of Capital | $ 1,802,913 | $ 5.64 |
| **Total General Expenses** | | | | **$ 2,236,574** | **$ 7.00** |
| **Total Product Cost** | **Sum of Manufacturing Costs and General expenses** | | | **$ 17,815,601** | **$ 56** |

**RF = Ratio factor**

Amount of $AlH_3$ produced per year 319,622 kg/yr

Ignore distribution and selling costs.

Ignore research and development costs.

# Model Details – Cartridge Cost Breakdown

- The cartridge costs are based on vendor and manufacturer estimates for the various cartridge components at two different production scales.
  - As production scale is increased, cost savings are realized through automation
- Estimates are provided for both newly manufactured and recycled cartridges
  - Assumes cartridge canisters, heaters, and insulation are recyclable
  - Recycling costs for emptying, cleaning, and prepping a cartridge is assumed equal to the filling costs.

| **Values in $/cartridge** | **Production Scale** | **4 M Cartridges/yr** | | **20 M Cartridges/yr** | |
|---|---|---|---|---|---|
| | **Basis** | **New** | **Recyled** | **New** | **Recyled** |
| **Recyclable components** | | | | | |
| cartridge cans/lids | Aluminum product manufacturer estimate | 0.75 | NA | 0.75 | NA |
| cartridge heater | Heater element vendor estimate | 0.50 | NA | 0.50 | NA |
| insulation | Insulation manufacturer estimate | 0.50 | NA | 0.50 | NA |
| **Consumable components** | | | | | |
| filters | Filter vendor estimate | 0.25 | 0.25 | 0.15 | 0.15 |
| stickers | Vendor estimate | 0.15 | 0.15 | 0.10 | 0.10 |
| powder filling | Metal powder products manufacturer estimate | 0.75 | 0.75 | 0.50 | 0.50 |
| **Components Total** | | **2.90** | **1.15** | **2.50** | **0.75** |
| **Labor** | | | | | |
| Handling, testing, & overhead | Estimate | 1.60 | 1.60 | 1.25 | 1.25 |
| Recycling (empty, clean, & prep) | Assumed equivalent to powder filling costs | NA | 0.75 | NA | 0.50 |
| **Labor Total** | | **1.60** | **2.35** | **1.25** | **1.75** |
| **TOTAL ($/CARTRIDGE)** | | **4.50** | **3.50** | **3.75** | **2.50** |
| **TOTAL ($/KG ALANE)** | | **53** | **41** | **44** | **29** |

Production scale: 4 M cartridges per year, equivalent to 320 MT/yr

Mass of alane per cartridge: 85 g