



# ***Chemical Hydride Slurry for Hydrogen Production and Storage***

**2005 DOE Hydrogen Program Review Presentation**

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# Overview

## Timeline

- Project start date: 1/1/04
- Work start: 4/1/04
- Project end date: 12/31/06
- Percent complete: 33%

## Budget

- Total project funding
  - DOE share: \$1.8M/ 3-4 years
  - Contractor share: \$457K
- Funding received in FY04: \$600K
- Funding for FY05: \$204K

## Barriers addressed for On-board storage

Project also applicable for Delivery, Off-board storage, and MgH<sub>2</sub> Cost reduction

- A. Cost
- B. Weight and Volume
- C. Efficiency
- G. Life Cycle and Efficiency Analyses
- R. Regeneration Processes
- S. Byproduct Removal
- T. Heat Removal

## Partners

- Hatch Technology, LLC
- Boston University
- Metallurgical Viability, Inc.
- HERA Hydrogen Storage Systems Inc.



# Objective and Approach

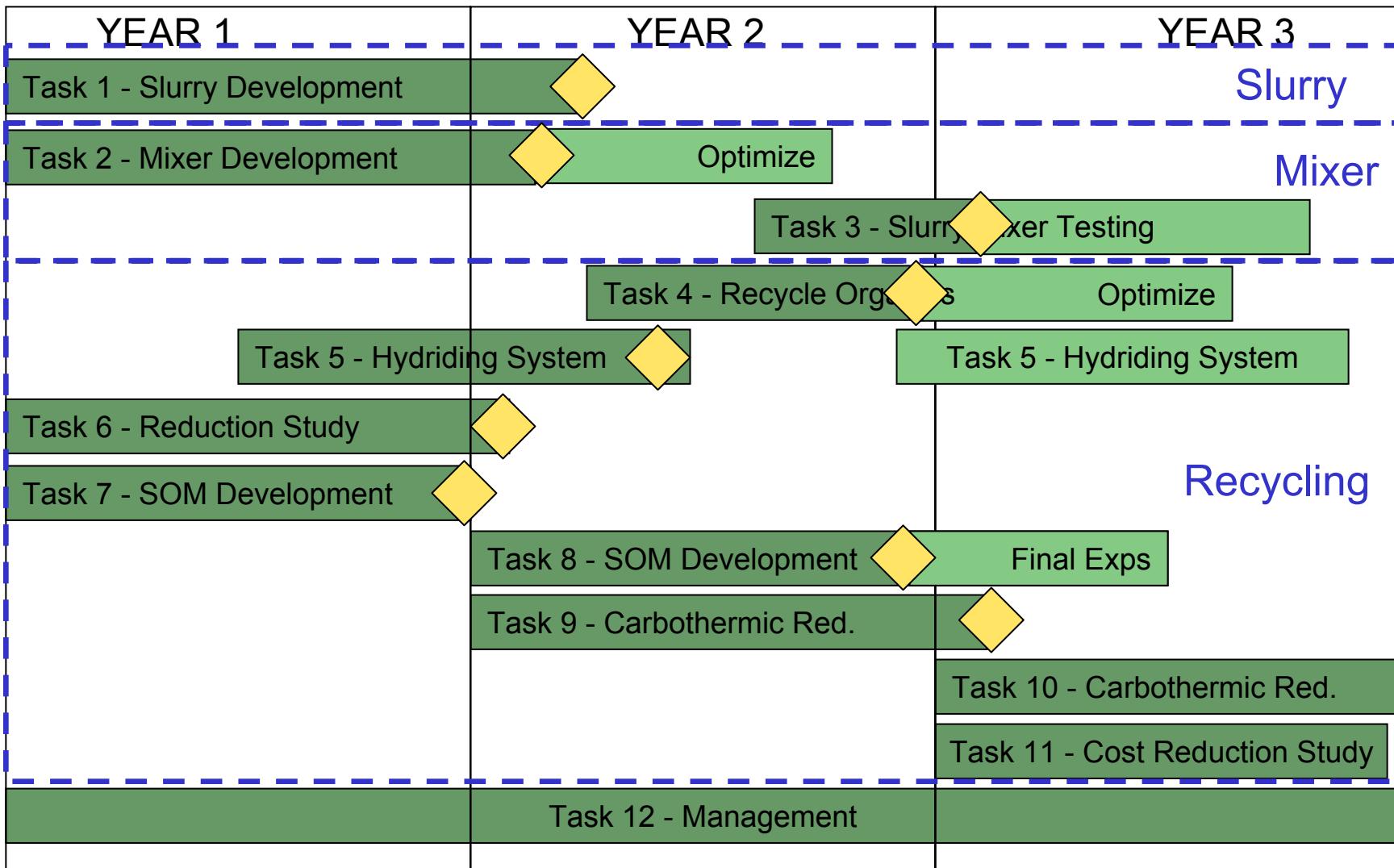
- **Objective** - Demonstrate that Magnesium Hydride Slurry is a cost effective, safe, and high-energy-density hydrogen storage, transportation, and production medium
  - Pumpable and high energy density slurry offers infrastructure advantages
  - High system energy density with high vehicle range
- **Approach**
  - **Slurry** - Develop a stable and very fluid MgH<sub>2</sub> slurry with slurry energy density of 3.9kWh/kg and 4.8kWh/L necessary for transportation and distribution
  - **Mixer** - Develop mixing system to use MgH<sub>2</sub> slurry and to meet 2kWh/kg and 1.5kWh/L system targets
  - **Cost** - Evaluate and develop Mg reduction and slurry production technologies to show potential cost of hydrogen, slurry, and system
    - Comparative evaluation of alternate Mg reduction technologies
    - Experimental Solid-oxide Oxygen-ion-conducting Membrane (SOM) process
    - Experimental carbothermic reduction process
    - Slurry production and component recycling
    - Mg hydriding, slurry mixing, Oil separation and recycle, Mg reduction



# PROJECT PLAN

◆ Go/No-Go

Year 1 began Apr 2004



# Issues and Options

- Issues that are being address in this project
  - Cost of: hydrogen from a *large scale* magnesium hydride slurry system
  - Cost of: reducing Mg, making MgH<sub>2</sub>, recovering the oils
  - Slurry stability: continued pumpability for lengthy storage and delivery to the market
  - Speed and control of hydrogen generation. Mixer needs to enable rapid reaction, with very compact and simple footprint to meet on board requirements
- Benefits of slurry technology
  - Slurry system can deliver hydrogen to the market with only slight modification to the existing transportation and delivery infrastructure.
  - Slurry based system can be used both as *fueling station* or an *on-board* storage and generation technology
  - Project Research will yield new magnesium and magnesium hydride production technology know-how which will benefit other metal based hydrogen storage technologies



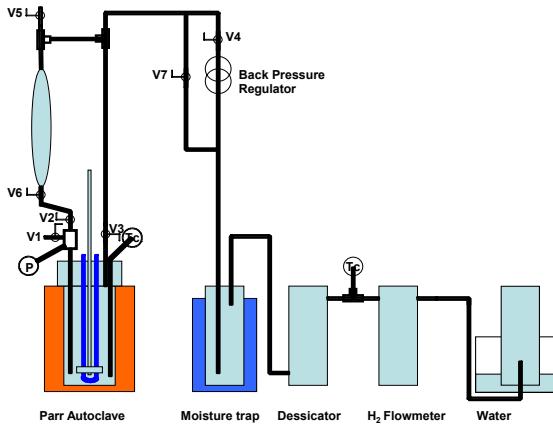
# Progress Slurry Development

*target: a pumpable slurry that stays liquid for months*

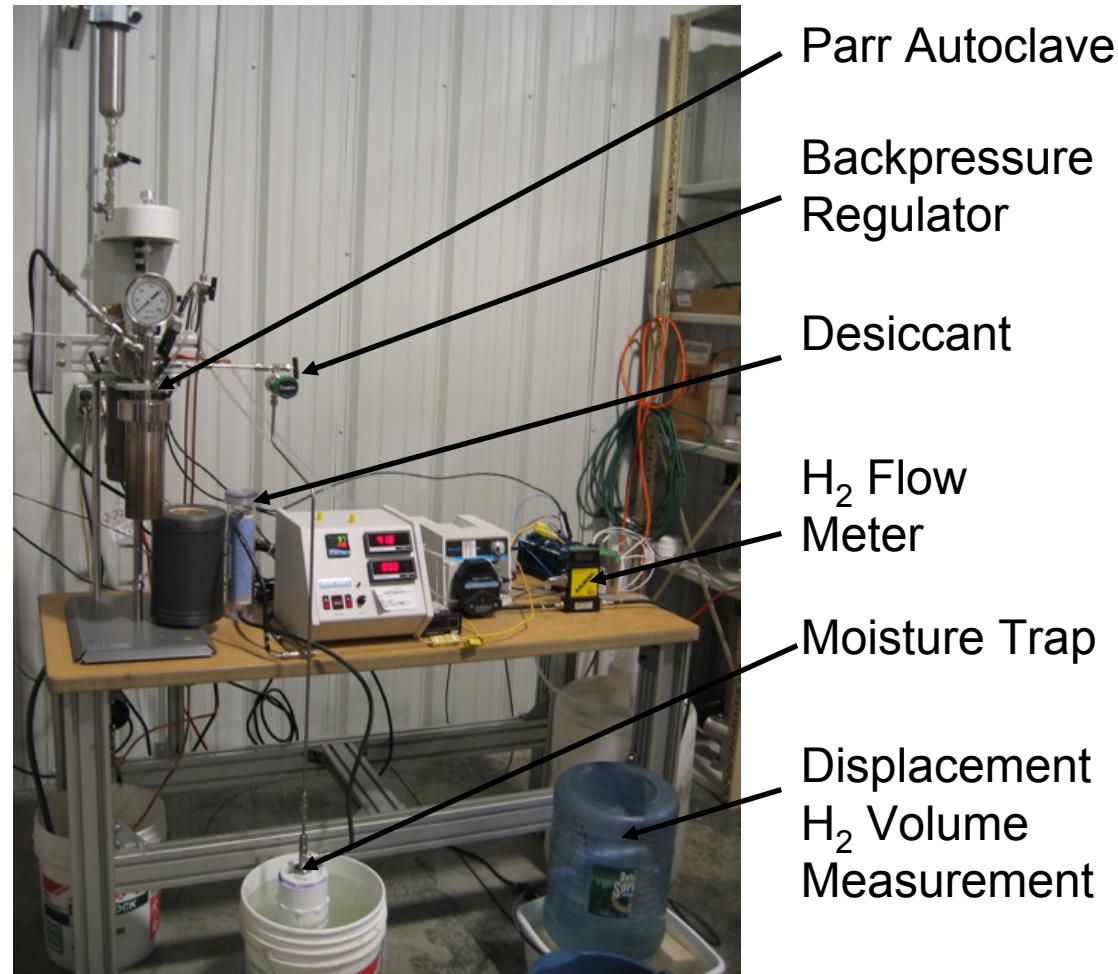
- Slurry characteristics depend on:
  - Carrier liquid and dispersant
  - Particle size, size mix and loading
- Completed tests of commercial MgH<sub>2</sub> powder with original dispersant
  - Partial success – but average particle size may be too large
- Have taken delivery of smaller particle size sample
  - Surface area 2.5 m<sup>2</sup>/gm
- Brought in slurry design experts: Dr. Alan Hatton of MIT and Jim McNamee of Uniqema (paint division of ICI chemical).
  - Tests using new dispersant and particle size mix showing improvements
- Evaluating particle size reduction alternatives
- **Significant achievements**
  - Current slurry is acceptable
  - Have developed confidence that improvements in energy density and stability are possible

# Progress :Mixer Development

*target: simple compact design providing efficient reaction control*



- 24 tests performed to date
  - Reaction rate
    - Reaction rate increases with temperature
    - Reaction rate self sustaining above 80°C
    - Rate is rapid enough for mixer application
  - Pumping
    - 24 hour pumping test
    - Early slurry showed some settling
  - Completion of reaction
    - 100% reaction observed





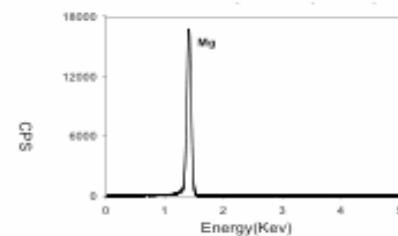
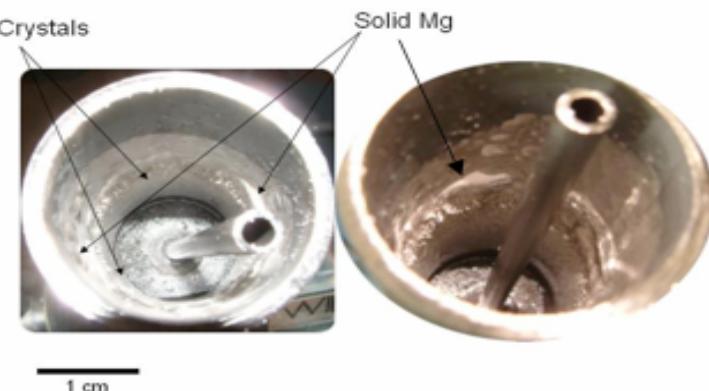
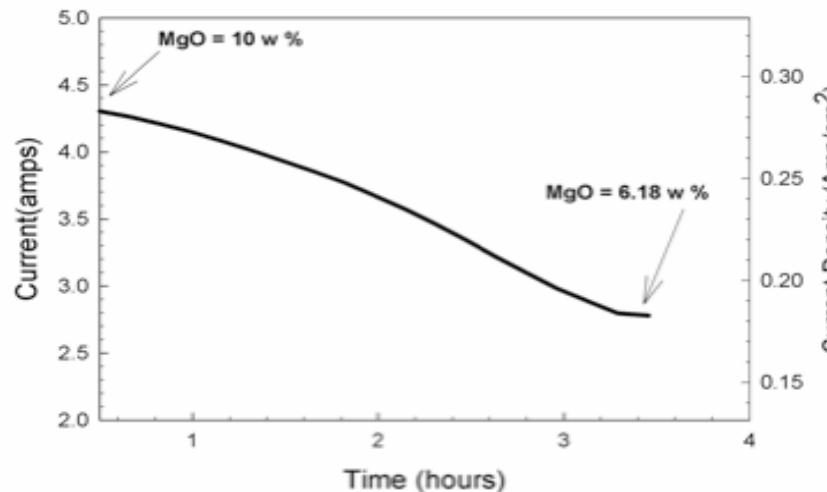
# Progress - Recycling

*Target: determine energy efficiencies and costs of alternative recycling processes*

- Three recycling studies are nearly complete
  - Carbothermic reduction
  - SOM reduction
  - MgCl<sub>2</sub> reduction
- Studies are providing bottom up analyses of the equipment, materials, and labor required for each process
- Process steps
  - Reclaim oil
  - Calcine Mg(OH)<sub>2</sub> to MgO
  - Reduce MgO to Mg
  - Hydride Mg + H<sub>2</sub> = MgH<sub>2</sub>
  - Mix slurry
- Preliminary Results
  - SOM appears to offer lowest energy consumption, reduction process can operate at 10 kWh/kg of Mg
  - Capital costs of carbothermic process considerably less than for MgCl<sub>2</sub> reduction

# Progress SOM

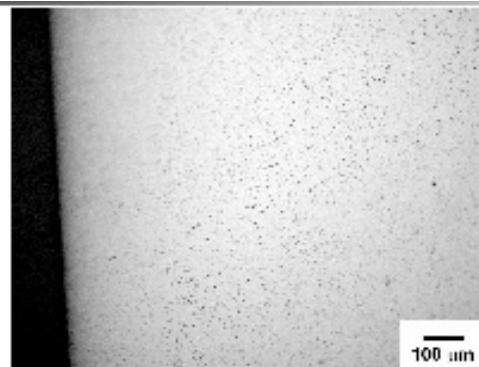
Have demonstrated temperature reduction  
from 1300°C to 1150°C



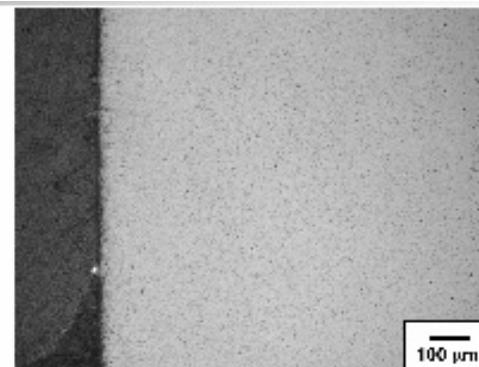
- Cell tested for 20 hours at 1150 °C
- Electrolysis at 3V, 39 Amp-hour passed, 18 g of Magnesium produced
- Pure Magnesium confirmed by EDAX analysis
- Faradic Efficiency of the process is high

# Progress SOM

## Stability of Membrane is excellent at 1150°C



a) As Received



b) After Experiment

- Membrane virtually unaffected after the 20 hour experiment
- Selection of flux is critical to the process
- The operating life of Zirconia membrane will dominate the overall cost of the process
  - Life of Zirconia membrane is significantly increased with lower temperature operation



# Questions from Last Meeting

- System Efficiency
  - Off-board regeneration efficiency
  - Life cycle efficiency
- Cost of Hydrogen
  - Preliminary costs based on material costs
- Component Mass/Volume
  - Due to high energy density of slurry and relatively fixed mass and volume of mixer system, energy density of slurry system improves as H<sub>2</sub> storage is increased



# Life Cycle Efficiency Comparison

## method of analysis

- Efficiency consuming steps considered
  - Production
  - Transportation to depot
  - Return transportation of truck and byproducts to production
  - Transportation to distribution station
  - Return Transportation of truck and byproducts to depot
  - Loading onto vehicle
- Reference calculation for comparison
  - Process efficiencies are consistent with preliminary H2A analysis results from NREL
  - Production and transportation of compressed hydrogen to fueling station
  - Production and transportation of liquid hydrogen to fueling station



# Preliminary Life Cycle Efficiency Comparison

Slurry matches LH<sub>2</sub> inefficiency with dramatic improvements in safety

Process	Efficiency (5000psi on-board)	(Hydrolysis on-board)
MgH <sub>2</sub> slurry with carbothermic reduction process Preliminary results requiring additional validation	33%	37%
MgH <sub>2</sub> slurry with SOM reduction process and electrolysis for hydrogen Preliminary results requiring additional validation	37%	41%
Liquid Hydrogen system starting with SMR	42%	
Liquid Hydrogen system starting with electrolysis H <sub>2</sub>	30%	
Compressed H <sub>2</sub> system starting with SMR	19%	
Compressed H <sub>2</sub> system starting with electrolysis H <sub>2</sub>	6%	

Liquid and compressed H<sub>2</sub> systems used results of H2A analysis  
References and assumptions in backup slides



# Sample process calculation

## Preliminary Analysis -*MgH<sub>2</sub> Slurry with SOM process*

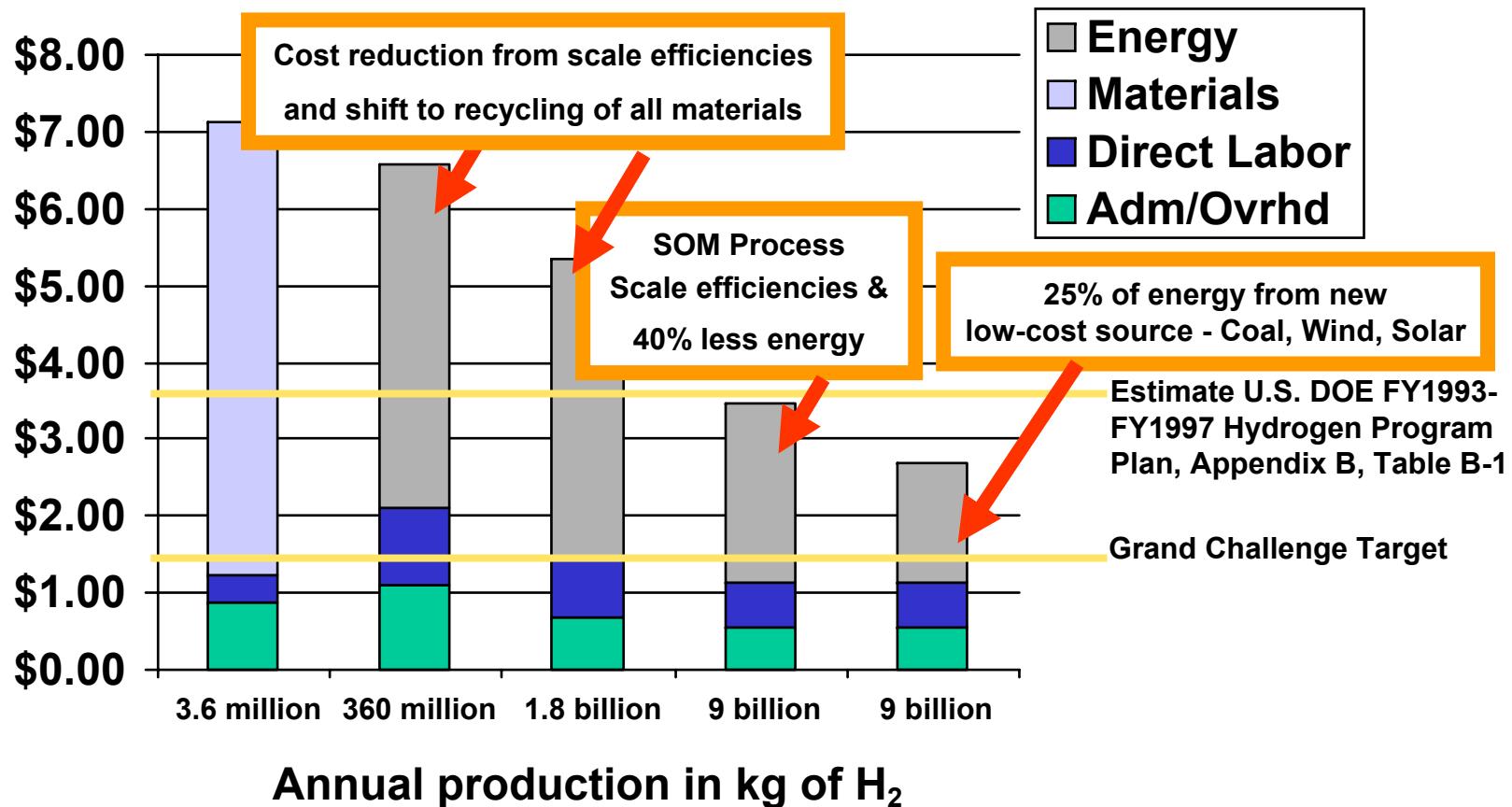
	Efficiency	Losses	Energy remaining
Start with 1 unit of energy			1.00
Recycle oils and dispersants	100.0%	1	-
SOM Reduction of Mg(OH)2 to MgH2	45.7%	2	0.54300
Add oils to make slurry	100.0%	-	0.46
Transport 500km to depot		0.01473	0.44
Return byproduct to production plant		0.01473	0.43
Transport 100km to distribution station		0.00835	0.42
Return byproduct to depot		0.00835	0.41
On-board hydrogen production		-	0.41
Hydrogen to fuel cell		-	0.41

1 - Recycle oils and dispersants using waste heat from SOM processes

2 - Hydrogen for MgH<sub>2</sub> from electrolysis

# PRODUCTION COST DRIVERS

## cost drivers shift from material to energy



- Detailed bottom up evaluation using Permanente Carbothermal Reduction model
- Top down evaluation using data about current costs of MgCl<sub>2</sub> reduction technology scaling to larger sizes
- Scale of processes required to support automotive application
- Materials cost evaluation

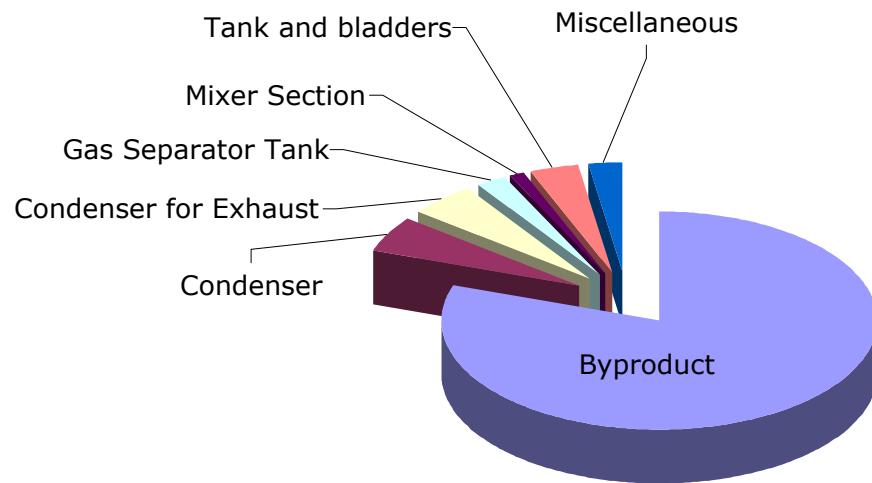


# HYDROGEN COST based on slurry materials costs

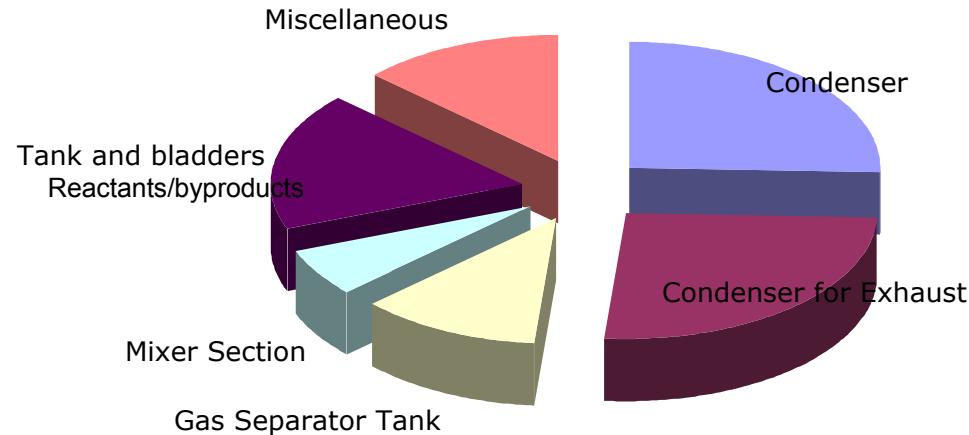
Item	Mass for 5 kg H <sub>2</sub>	Current Cost of Material	Cost of slurry using small scale hydride production	Cost of slurry using metal and hydrogen	Anticipated material costs yielded in recycling
	kg	\$/kg	\$	\$	\$
Mg	30.15	2.76		83.21	Produced in process
H <sub>2</sub>	2.5	6.67		16.68	Produced in process
MgH <sub>2</sub>	32.65	250.00	8162.50	99.89	9.05
Oil	9.86	1.11	10.91	10.91	0.55
Dispersant	0.30	14.41	4.32	4.32	0.22
Slurry	42.81		8177.73	115.12	9.82
H <sub>2</sub> Produced	5.0		\$1,636/kg	\$23/kg	\$2/kg Meets target

# Breakdown of Mass and Volume of Mixer for Condensing Fuel Cell Exhaust

## Mass Breakdown



## Volume Breakdown

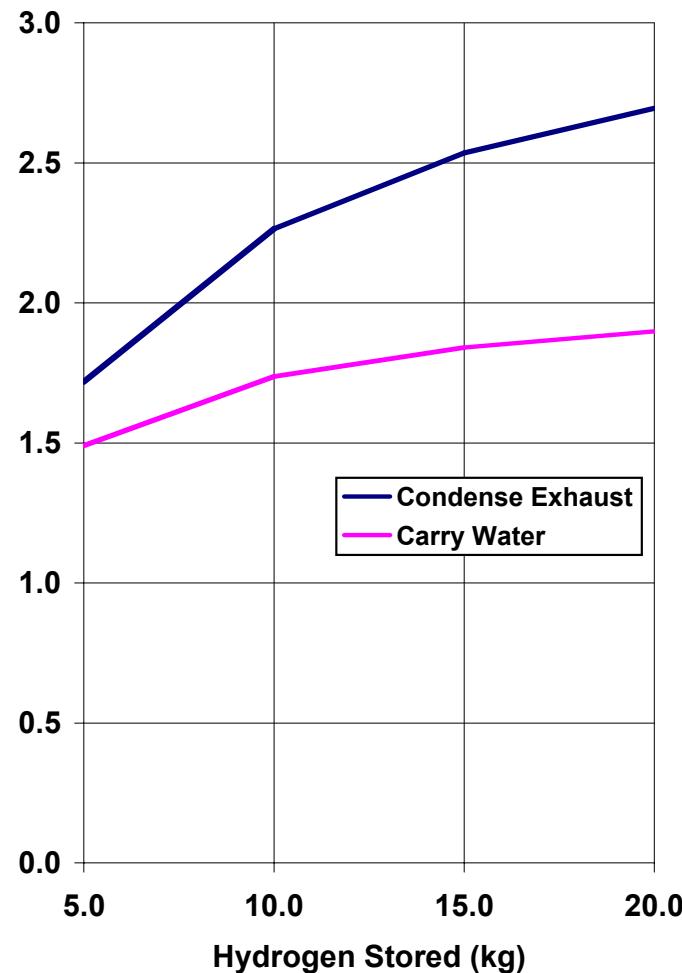
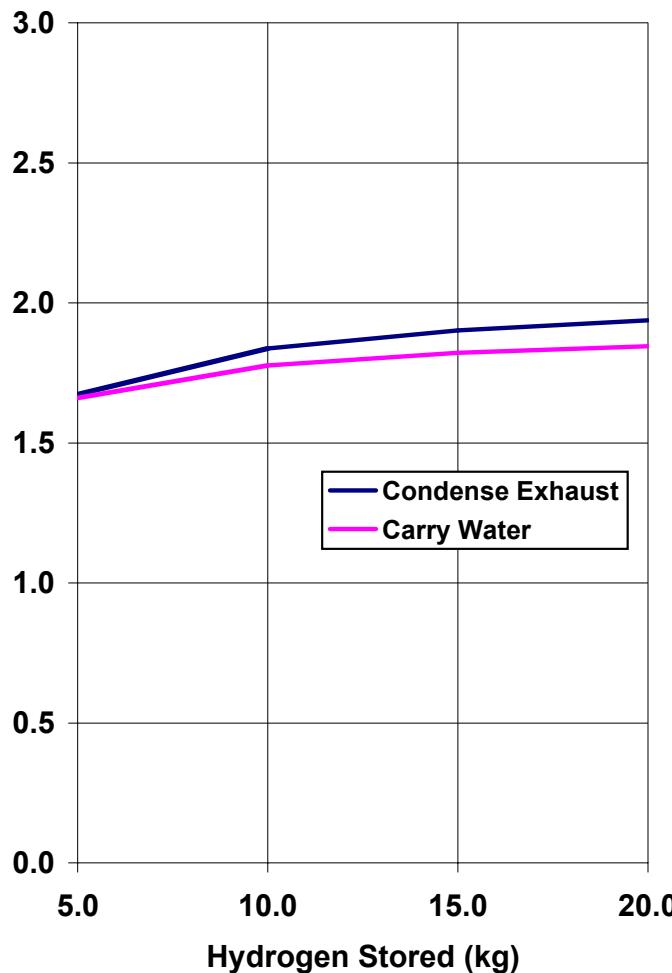


- Mass and volume of tanks and bladders calculated from estimates of mass and volume of slurry, water, byproduct, steel, and bladder material
- Mass and volume of condenser and mixer system based on original LiH slurry system
- Mass and volume of additional components estimated with the assumption that components will be built specifically for this application
- Condensing system is heaviest when hydrogen is consumed thus showing byproduct in mass breakdown
- Slurry/Water/Byproduct are within the Tank and Bladder volume in the Volume Breakdown
- Detailed listing in backup slide



# Energy Density

Slurry approach has higher energy density when  
more hydrogen is stored





# Accomplishments

- Prepared slurry with acceptable stability and energy density
- Demonstrated that slurry/water reaction is fast enough for mixer at appropriate conditions
  - 100% of hydrogen expected has been measured
- Mg reduction process studies nearing completion
  - Cost reductions in simplified process and use of large scale
  - Cost of process looks attractive
- SOM process development making significant improvements
  - Process operation at 1150°C with minimum wear on membrane promises low costs of operation and maintenance
  - Continued high energy efficiency <10 kWh/kg Mg



# Future Work

- FY05
  - Go/No-go decisions
    - Reduction study, SOM, Slurry, Mixer development
  - Mixer prototype
  - Expansion of Recycle Studies
  - Improve slurry stability
  - Begin hydriding evaluation
  - Focus SOM development on
    - Production of MgH<sub>2</sub> in SOM condenser
    - Use of byproduct Mg(OH)<sub>2</sub> as the input to SOM
- FY06 Plans
  - Scale-up experiments of SOM process
  - Testing of slurry and mixer for robustness and hydrogen purity
  - Complete hydriding evaluation
  - Recycle organics evaluation



# Backup Slides



# Supplementary Slides



# Publications and Presentations from the past year

- 3. Andrew W. McClaine, "Chemical Hydride Slurry for Hydrogen Production and Storage", 2004 DOE Hydrogen, Fuel Cells & Infrastructure Technologies Program Review, Philadelphia, PA, 25 May 2004
- 4. Andrew W. McClaine, Safety Discussion, prepared for the 2004 DOE Hydrogen, Fuel Cells & Infrastructure Technologies Program Review, Philadelphia, PA, 25 May 2004
- 5. Kenneth Brown, "Chemical Hydride Slurry for Hydrogen Storage", presented at the "Hydrogen Generation & Storage Systems session" of the Hydrogen and Fuel Cells Summit, Worcester Polytechnic Institute, October 20, 2004.
- 6. Andrew W. McClaine, "Chemical Hydride Slurry for Transportation Applications" presented at the "Transportation Applications and Challenges Session" of the Hydrogen and Fuel Cells Summit, Worcester Polytechnic Institute, October 20, 2004.
- 7. Ajay Krishnan, Xionggang Lu, Srikanth Gopalan, Uday B Pal of Manufacturing Engineering, Boston University, Brookline, Massachusetts and Andrew W McClaine of Safe Hydrogen LLC, Lexington, Massachusetts, "Magnesium-Hydride Slurry Technology for Hydrogen Storage", Materials Research Society, Hynes Convention Center & Sheraton Hotel, Boston, MA, 2 December 2004
- 8. Ajay Krishnan, Xionggang Lu, Srikanth Gopalan, Uday B Pal, of Boston University, and Andrew W McClaine of Safe Hydrogen, LLC, "Magnesium-Hydride Slurry Technology for Hydrogen Storage", Presentation at the Materials Research Society Fall Meeting, Boston, MA, 29 November-3 December 2005
- 9. Robert R. Odle of Metallurgical Viability, Inc., Andrew W. McClaine of Safe Hydrogen, LLC, and Jens Frederiksen of PF&U Mineral Development ApS, "Economic Analysis of the Carbothermal Production of Magnesium", TMS2005 134th TMS Annual Meeting Magnesium Technology 2005, San Francisco, CA, February 13-17, 2005
- 10. Ajay Krishnan, X. Lu, and U.B. Pal of Boston University Manufacturing Engineering Department, "Solid Oxide Membrane (SOM) for Cost Effective and Environmentally Sound Production of Magnesium Directly from Magnesium Oxide", TMS2005 134th TMS Annual Meeting Magnesium Technology 2005, San Francisco, CA, February 13-17, 2005
- 11. K. Brown, "Chemical Hydride Slurry for Hydrogen Production and Storage", DOE FreedomCAR - Hydrogen Storage Tech Team Annual Review, Houston, TX, 24 February 2005



# Hydrogen Safety

Most significant hazard associated with this project

- Safety is an inherent feature of MgH<sub>2</sub> slurry
  - Reaction of MgH<sub>2</sub> and water is very slow at room temperature
  - No gaseous hydrogen is present unless it is desired
  - Byproduct of the reaction is not hazardous “Milk of Magnesia”
  - Slurry and byproduct are stored at normal pressure and temperatures
- Most significant hazard is the ignition of gaseous hydrogen during experiments
  - Hydrogen produced is contained within production vessel or within measurement volume
  - Currently using a water displacement method and a hydrogen flowmeter to measure hydrogen production



# Hydrogen Safety

Our approach to deal with this hazard

- Methods of minimizing hazard
  - Work with small quantities of hydrogen
    - Quantity in bottle is less than 15L (1.35g H<sub>2</sub>) (equivalent to a teaspoon of gasoline)
  - Dilution of hydrogen with air to levels less than 2 vol% when quantities produced are large
    - Requires mixing a flow rate of 10L/min of H<sub>2</sub> with 500 L/min (19 scfm) of air
    - Vent hydrogen into flow of compressed air at appropriate flow rate
    - Vent to exterior of building
  - Support bottle well to prevent spillage
  - Minimize combustion sources near experiment



# Life Cycle Efficiency Calculations



# Life Cycle Efficiency Comparison

## method of analysis

- Efficiency consuming steps considered
  - Production
  - Transportation to depot
  - Return transportation of truck and byproducts to production
  - Transportation to distribution station
  - Return Transportation of truck and byproducts to depot
  - Loading onto vehicle
- Reference calculation for comparison
  - Process efficiencies are consistent with preliminary H2A analysis results from NREL
  - Production and transportation of compressed hydrogen to fueling station
  - Production and transportation of liquid hydrogen to fueling station



# Efficiency Calculation for MgH<sub>2</sub>

## Slurry with SOM process

for delivering H2 to station

		Efficiency	Losses	Energy remaining
Start with 1 unit of energy				1.00
Recycle oils and dispersants		100.0%	-	1.00
SOM Reduction of Mg(OH)2 to MgH2	1	45.7%	0.54300	0.46
Add oils to make slurry		100.0%	-	0.46
Transport 500km to depot			0.01473	0.44
Return byproduct to production plant			0.01473	0.43
Transport 100km to distribution station			0.00836	0.42
Return byproduct to depot			0.00836	0.41
Compress to 5000 psi from 200 psi			0.04000	0.37
Hydrogen to fuel cell			-	0.37

1 - SOM process is assumed to use electrolysis to provide the hydrogen for the MgH<sub>2</sub>

# Analysis Notes

- MgO to Mg reduction proven at 10kWh/kg Mg in SOM process. Theoretical max is 6.87kWh/kg Mg.
- Liquid pump losses are neglected
- 500 km trucking
  - 1000 km round trip,  $39.2\text{L}_{\text{diesel}}/100\text{km}$ ,  $\text{LHV}_{\text{diesel}}=35.8\text{MJ/L}$  (H2A study)
  - Slurry truck capacity = 3973 kg H<sub>2</sub>
  - Compressed H<sub>2</sub> truck capacity = 340.1 kg H<sub>2</sub> (H2A study)
  - Liquid H<sub>2</sub> truck capacity = 4142 kg H<sub>2</sub> (H2A study)
- 100 km trucking
  - 200 km round trip,  $28\text{L}_{\text{diesel}}/100\text{km}$ ,  $\text{LHV}_{\text{diesel}}=35.8\text{MJ/L}$  for slurry truck
  - Slurry truck capacity = 1000 kg H<sub>2</sub>
  - 200 km round trip,  $39.2\text{L}_{\text{diesel}}/100\text{km}$ ,  $\text{LHV}_{\text{diesel}}=35.8\text{MJ/L}$  for liquid and compressed hydrogen (H2A study)
  - Compressed H<sub>2</sub> truck capacity = 340.1 kg H<sub>2</sub> (H2A study)
  - Liquid H<sub>2</sub> truck capacity = 4142 kg H<sub>2</sub> (H2A study)



# Analysis Notes Continued

- Estimates of compression energy taken from H2A study and compared to calculations of adiabatic and isothermal compression energy. Actual assumed to be halfway between adiabatic and isothermal. This is consistent with data from two existing hydrogen compressors.
- When pumping down a tank, compression energy estimated to be half that of compressing from low to high pressure values
- H<sub>2</sub> liquefaction energy estimated to be 32.4% of the H<sub>2</sub> LHV at present based on H2A study.
- H<sub>2</sub> compression at 180 bar (2640 psi) for truck transportation and 410 bar (6,000 psi) for storage at production, depot, and distribution station per H2A study.
- H<sub>2</sub> venting losses during LH<sub>2</sub> transportation - 0.5%/day. No losses assumed at distribution station since H<sub>2</sub> sales assumed to be high enough to consume H<sub>2</sub> gas
- Transfer losses assumed to be 6% for LH<sub>2</sub> per H2A study. Assumed captured and re-condensed for depot and captured and compressed to 6000psi for station
- H<sub>2</sub> produced by Steam Methane Reformation at 85% efficiency. Hydrogen produced for the MgH<sub>2</sub> slurry in carbothermic process is part of the system and in SOM process is produced by electrolysis.
- H<sub>2</sub> produced by electrolysis at 61.2% efficiency based on Hydrogenics public data and the LHV of H<sub>2</sub>. The reaction  $2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O}$  produces about 33.3kWh/kg H<sub>2</sub>. The current published data claims 54.5kWhr/kg H<sub>2</sub>.



# Efficiency Calculation for Liquid Hydrogen with SMR process

	Efficiency	Losses	Energy remaining
Produce H <sub>2</sub> with SMR	85.0%	0.15000	0.85
Liquify H <sub>2</sub> produced	67.6%	0.32400	0.53
Liquid storage losses captured and reliquified		0.00081	0.53
Pump from storage tank to truck	100.0%	-	0.53
Transport 500km to depot		0.01413	0.51
Vent loss from truck		0.00500	0.51
Truck unloading losses assumed captured & condensed		0.01944	0.49
Return truck to production plant		0.01413	0.47
Transport 100km to distribution station		0.00215	0.47
Vent loss from truck		0.00500	0.47
Truck unloading losses assumed captured & compressed		0.00648	0.46
Return truck to depot		0.00215	0.46
Liquid to 5000 psi - vaporizing energy		0.03260	0.42
Hydrogen to fuel cell		-	0.42



# Efficiency Calculation for Liquid Hydrogen with Electrolysis H<sub>2</sub>

	Efficiency	Losses	Energy remaining
Produce H2 with Electrolysis	61.2%	0.38800	0.61
Liquify H2 produced	67.6%	0.32400	0.29
Liquid storage losses captured and reliquified		0.00081	0.29
Pump from storage tank to truck	100.0%	-	0.29
Transport 500km to depot		0.01413	0.27
Vent loss from truck		0.00500	0.27
Truck unloading losses assumed captured & condensed		0.01944	0.25
Return truck to production plant		0.01413	0.23
Transport 100km to distribution station		0.00215	0.23
Vent loss from truck		0.00500	0.23
Truck unloading losses assumed captured & compressed		0.00648	0.22
Return truck to depot		0.00215	0.22
Liquid to 5000 psi - vaporizing energy		0.03260	0.19
Hydrogen to fuel cell		-	0.19



# Efficiency Calculation for Compressed Hydrogen with Electrolysis H<sub>2</sub>

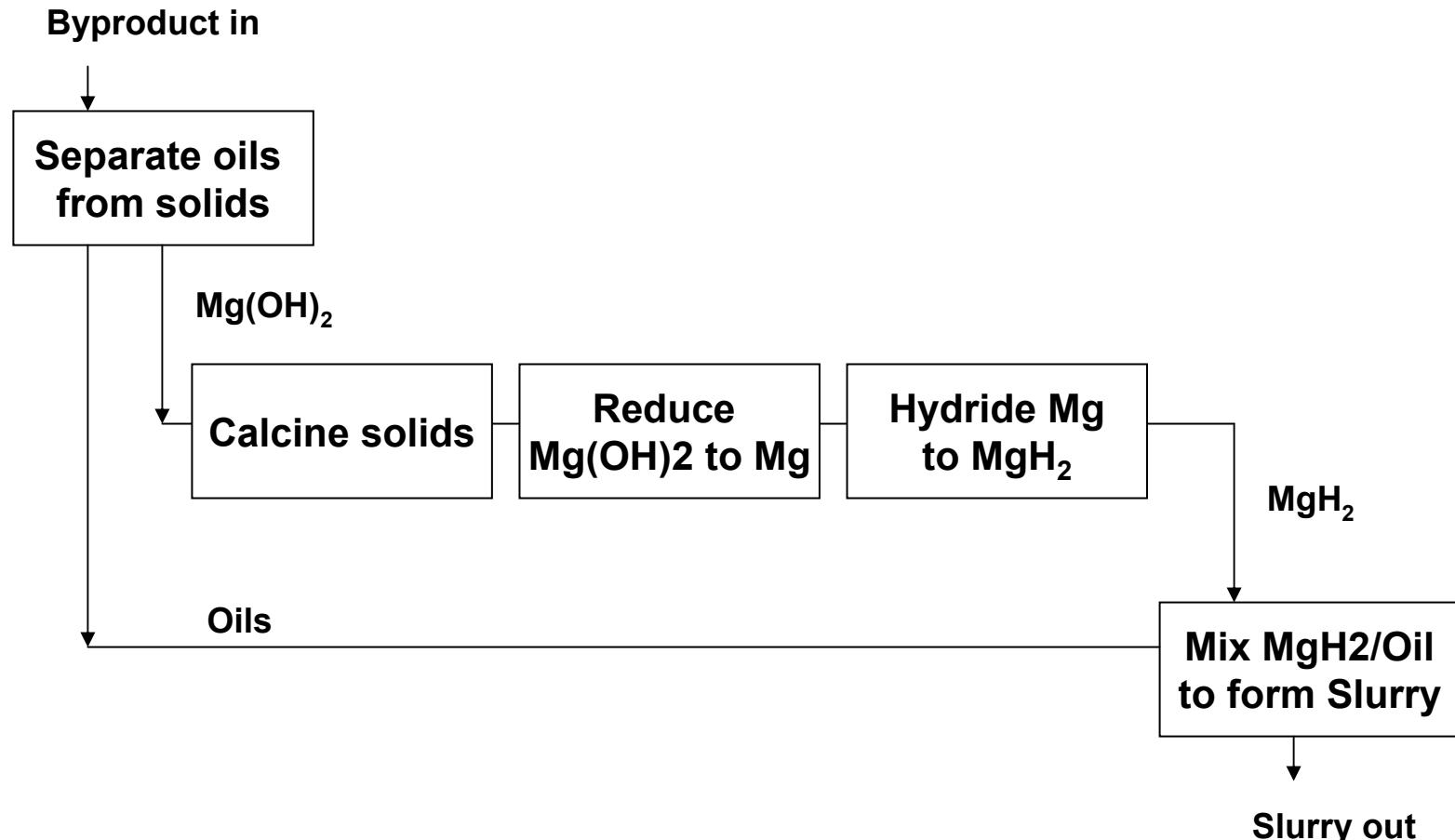
	Efficiency	Losses	Energy remaining
Produce H <sub>2</sub> with Electrolysis	61.2%	0.38800	0.61
Compress from 300 psi to 6000 psi		0.06700	0.55
Compress from storage tank to truck		-	0.55
Transport 500km to depot		0.17206	0.37
Compress from truck to storage at depot	0.963	0.03700	0.34
Return truck to production plant		0.17206	0.16
Compress from storage tank to truck		-	0.16
Transport 100km to distribution station		0.03441	0.13
Compress from truck to storage at station	0.963	0.03700	0.09
Return truck to depot		0.03441	0.06
Compress to 5000 psi tank on vehicle		-	0.06
Hydrogen to fuel cell		-	0.06



# Recycling - Process Efficiency Calculation

# Progress - Recycling

## Efficiency Calculation from Mass and Energy Balance





# MgH<sub>2</sub> slurry process steps

## SOM Process Summary

Flow rate Mg	kg/hr	2,511
Flow rate H <sub>2</sub> from slurry	kg/hr	416
Flow Mg/Flow H <sub>2</sub>		6

Process Step		delta H kJ/kg H <sub>2</sub>	delta G kJ/kg H <sub>2</sub>	Tin K	Tout K
Calcine - heat reactants	Mg(OH) <sub>2</sub> , air	18,519	(5,555)	298	700
Calcine - Mg(OH) <sub>2</sub> to MgO	Mg(OH) <sub>2</sub> + Air = MgO + H <sub>2</sub> O + Air	40,701	(101,451)	700	700
SOM Heat reactants	MgO, Ar, H <sub>2</sub>	21,776	(99,166)	700/298	1423
SOM reaction	MgO = Mg + O	245,411	148,494	1423	1423
SOM reaction	H <sub>2</sub> + O = H <sub>2</sub> O	(127,197)	(58,670)	1423	1423
Cool Products	Mg, Ar	(41,407)	35,760	1423	800
Cool Products	Mg, Ar	(1,500)	5,321	800	523
Cool Products	H <sub>2</sub> O	(3,922)	14,191	1423	800
Hydride	Mg(s) + H <sub>2</sub> = MgH <sub>2</sub>	(19,526)	(1,488)	523	523
Electrolytic H <sub>2</sub>	2H <sub>2</sub> O = 2H <sub>2</sub> + O <sub>2</sub>	140,176	109,632	400	400
Hydrolysis	MgH <sub>2</sub> + 2H <sub>2</sub> O = 2H <sub>2</sub> + Mg(OH) <sub>2</sub>	(61,222)	(92,896)	298.15	400



# Reduction

## Positive delta G typical of electrolytic processes that use thermal and electrical inputs

		n moles/hr	mass kg/hr	delHf298 kJ/mole	T K	delH kJ/mole	S J/moleK	H kJ	delG kJ
<b>SOM Reduction</b>									
$MgO = Mg + O$									
MgO (s)	92	103,266	4,163	-601.2408	1423	55.122	100.695	(56,395,573)	(71,192,471)
Ar	94	82,613	3,300	0	1423	23.381128	187.332	1,931,583	(20,090,778)
Mg(g)	104	103,266	2,511	147.1002	1423	23.381	181.135	17,604,933	(9,012,438)
Ar	105	82,613	3,300	0	1423	23.381128	187.332	1,931,583	(20,090,778)
O	105	103,266	1,652	249.1731	1423	23.696415	194.162	28,178,178	(353,419)
HR			7,463					(54,463,990)	(91,283,249)
Pelectric in	in							58,285,671	
Heat in								43,893,013	
HP			7,463					47,714,694	(29,456,634)
Qrecovery								-	
Qloss									
Q=Hp+Qloss-Hr-Pelectric			(0)					(0)	61,826,614
<b>SOM Reduction</b>									
$O + H_2 = H_2O$									
H2	214	103,266	208.178	0	1423	31.965	177.153	3,300,902	(22,731,324)
O	109	103,266	1,652.196	249.1731	1423	23.696415	194.162	28,178,178	(353,419)
H2O(g)		103,266	1,860	-241.826	1423	33.816072	177.153	(21,480,379)	(47,512,586)
HR			1,860					31,479,080	(23,084,743)
Pelectric in									
HP			1,860					(21,480,379)	(47,512,586)
Qrecovery								52,959,459	
Qloss									
Q=Hp+Qloss-Hr-Pelectric			(0)					(0)	(24,427,844)



# Efficiency of MgH<sub>2</sub> System Using All Electric SOM Process

Energy input as electricity for SOM	kJ/hr	58,285,671
Energy input as electricity for H <sub>2</sub> electrolysis	kJ/hr	50,962,020
Energy produced as stored hydrogen	kJ/hr	49,944,951
Efficiency		0.457



# Calcination

## Mass and Energy Evaluation

	n moles/hr	mass kg/hr	delHf298 kJ/mole	T K	delH kJ/mole	S J/moleK	H kJ	delG kJ
Calcination								
$Mg(OH)_2 + CO + O_2 = MgO + H_2O + CO_2$								
Mg(OH) <sub>2</sub> (s)	103,266	6,023.176	-924.664	700	39.11514	144.529	(91,447,200)	(101,894,659)
O <sub>2</sub>	90,000	2,880	0	700	12.587	231.610	1,132,869	(13,458,552)
N <sub>2</sub>	338,400	9,480	0	700	12.009	216.956	4,063,819	(47,328,603)
MgO (s)	103,266	4,163	-601.2408	700	17.995	64.456	(60,229,534)	(64,888,819)
H <sub>2</sub> O(g)	out	103,266	1,860	700	14.191	218.737	(23,506,985)	(39,318,670)
CO <sub>2</sub>	out	0	-	700	17.754	250.752	-	-
O <sub>2</sub>	out	90,000	2,880	0	700	12.587	231.610	1,132,869
N <sub>2</sub>	out	338,400	9,480	0	700	12.009	216.956	4,063,819
HR		18,383					(86,250,513)	(162,681,814)
Recovered heat in							7,710,681	
HP		18,383					(78,539,831)	(164,994,645)
Qloss							-	
Q=Hp+Qloss-Hr-Pelectric		-					0	(2,312,831)



# Hydriding

## Mass and Energy Evaluation

		n moles/hr	mass kg/hr	delHf298 kJ/mole	T K	delH kJ/mole	S J/moleK	H kJ	delG kJ
Hydriding process									
$Mg + H_2 = MgH_2$									
Mg(s)	154	103,266	2,511	0	523	5.898	47.345	609,064	(1,947,954)
Ar	155	82,613	3,300	0	523	4.6737281	166.526	386,110	(6,808,906)
H <sub>2</sub>	156	103,266	208	0	523	6.555	147.054	676,909	(7,265,210)
MgH <sub>2</sub> (s)		103,266	2,719	-76.14922	523	9.8744238	55.342	(6,843,941)	(9,832,843)
Ar	out	82,613	3,300	0	523	4.6737281	166.526	386,110	(6,808,906)
H <sub>2</sub>	214	0	-	0	523	6.555	147.054	-	-
HR			6,019					1,672,083	(16,022,070)
Pelectric in									
HP			6,019					(6,457,831)	(16,641,748)
Qloss									
Qheat trans fluid					523			8,129,915	
Q=Hp+Qloss-Hr-Pelectric			0					0	(619,679)



# H<sub>2</sub>O Electrolysis

Positive delta G typical of electrolytic processes that use thermal and electrical inputs

		n moles/hr	mass kg/hr	delHf298 kJ/mole	T K	delH kJ/mole	S J/moleK	H kJ	delG kJ
Electrolytic hydrogen production $\text{H}_2\text{O(l)} = \text{H}_2 + \text{O}_2$									
H <sub>2</sub> O (l)	199	206,532	3,721	-285.8304	400	7.711453	92.189	(57,440,497)	(65,056,529)
O <sub>2</sub>	out	103,266	3,304	0	400	3.018	213.820	311,621	(8,520,528)
H <sub>2</sub>	152	103,266	208	0	400	2.959	139.215	305,564	(5,444,910)
H <sub>2</sub>	121	103,266	208	0	400	2.959	139.215	305,564	(5,444,910)
HR			3,721					(57,440,497)	(65,056,529)
Power in								50,962,020	
Heat in								9,592,851	
HP			3,721					922,749	(19,410,347)
Qloss								2,191,624	
Qheat trans fluid					400				
Q=Hp+Qloss-Hr-Pelectric			0					(0)	45,646,182



# MgH<sub>2</sub> Hydrolysis

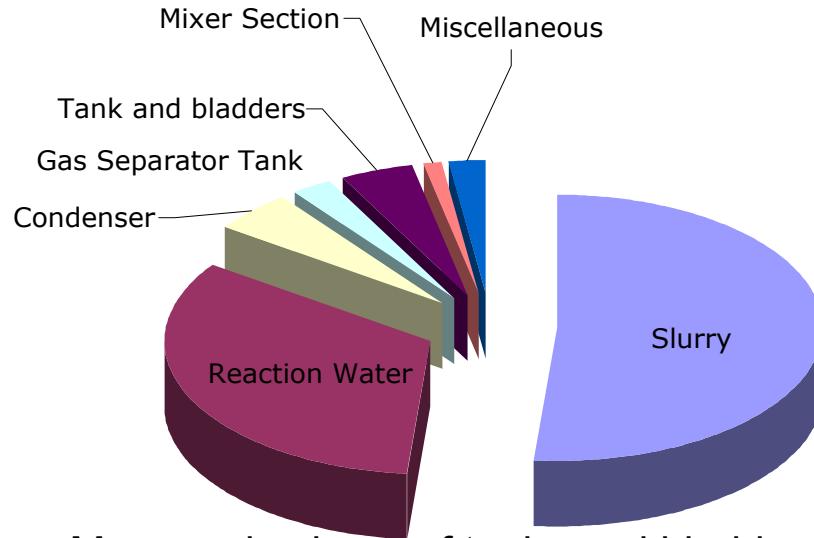
	n moles/hr	mass kg/hr	delHf298 kJ/mole	T K	delH kJ/mole	S J/moleK	H kJ	delG kJ
Hydrolysis								
$\text{MgH}_2 + (x+2)\text{H}_2\text{O} = \text{Mg(OH)}_2 + 2\text{H}_2 + (y)\text{H}_2\text{O(l)} + (x-y)\text{H}_2\text{O(g)}$								
MgH <sub>2</sub> (s)	171	103,266	2,719	-76.14922	298.15	0	31.032	(7,863,635)
H <sub>2</sub> O(l)	In	206,532	3,721	-285.8304	298.15	0	69.954	(59,033,196)
2 H <sub>2</sub> O(l)	266	206,532	3,721	-285.8304	298.15	0	69.954	(59,033,196)
Mg(OH) <sub>2</sub> (s)	244	103,266	6,023	-924.664	400	8.674	88.157	(94,590,739)
H <sub>2</sub>	489	206,532	416	0	400	2.959	139.215	611,129
1 H <sub>2</sub> O(l)	264	206,532	3,721	-285.8304	400	7.711453	92.189	(57,440,533)
H <sub>2</sub> O(g)	255	0	-	-241.826	400	3.452	198.789	(65,056,569)
Hr			10,160					(125,930,028)
H <sub>p</sub>			10,160					(174,178,587)
Q <sub>loss</sub>							25,490,115	
Q=H <sub>p</sub> +Q <sub>loss</sub> -H <sub>r</sub>			-				0	(38,677,924)



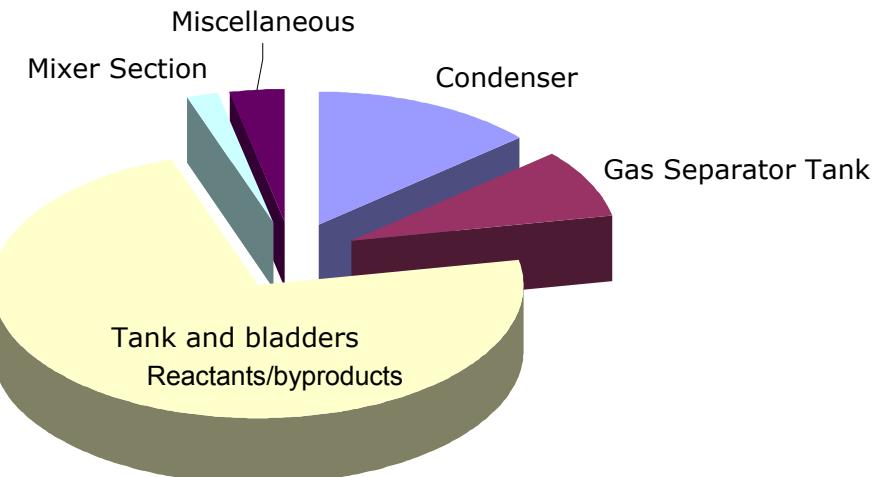
# Mixer System Component Breakdown

# Breakdown of Mass and Volume of Mixer for Carrying Reaction Water

## Mass Breakdown



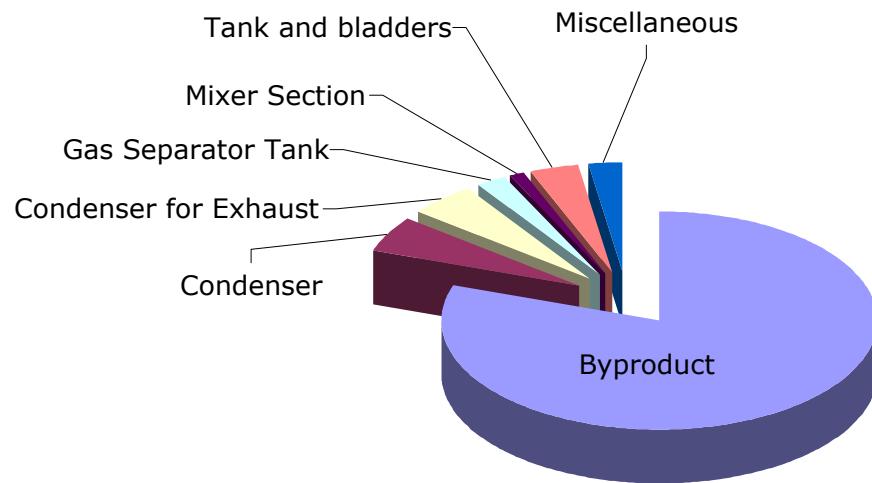
## Volume Breakdown



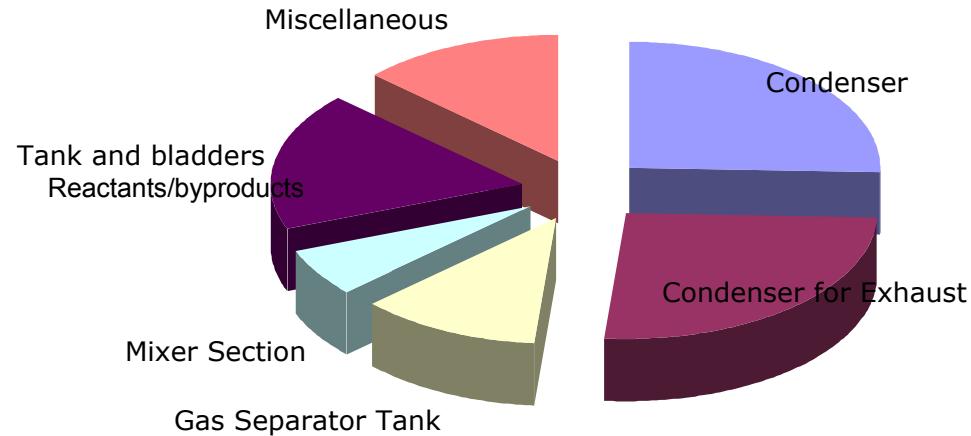
- Mass and volume of tanks and bladders calculated from estimates of mass and volume of slurry, water, byproduct, steel, and bladder material
- Mass and volume of condenser and mixer system based on original LiH slurry system
- Mass and volume of additional components estimated with the assumption that components will be built specifically for this application
- Condensing system is heaviest when hydrogen is consumed thus showing byproduct in mass breakdown
- Slurry/Water/Byproduct are within the Tank and Bladder volume in the Volume Breakdown
- Detailed listing in backup slide

# Breakdown of Mass and Volume of Mixer for Condensing Fuel Cell Exhaust

## Mass Breakdown



## Volume Breakdown



- Mass and volume of tanks and bladders calculated from estimates of mass and volume of slurry, water, byproduct, steel, and bladder material
- Mass and volume of condenser and mixer system based on original LiH slurry system
- Mass and volume of additional components estimated with the assumption that components will be built specifically for this application
- Condensing system is heaviest when hydrogen is consumed thus showing byproduct in mass breakdown
- Slurry/Water/Byproduct are within the Tank and Bladder volume in the Volume Breakdown
- Detailed listing in backup slide



# SPECIFIC ENERGY DETAIL

## Comparing H<sub>2</sub> storage and exhaust condensing vs carrying water

H2 Stored (kg) H2 Peak Flow Rate (kg/hr)	Condense Exhaust				Carry water				Condense Exhaust				Carry water			
Item	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L	Mass kg	System Volume L
Fuel Tank	1.5	51.4	1.9	81.4	2.2	101.5	2.9	161.4	3.3	201.7	4.5	320.8				
Balloons or bladders for water	0.2		0.8		0.3		1.1		0.5		1.7					
Balloons or bladders for slurry	0.9		0.9		1.3		1.3		2.0		2.0					
Balloons or bladders for byproduct	0.9		0.9		1.3		1.3		2.0		2.0					
Fuel/Water Pump	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3				
Heater	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1				
Mixer Section	1.2	2.3	1.2	2.3	1.2	2.3	1.2	2.3	1.2	2.3	1.2	2.3				
Mixer motor/stirrer	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3				
Gas Separator Tank	2.3	9.4	2.3	9.4	2.3	9.4	2.3	9.4	2.3	9.4	2.3	9.4				
Separator Mixer Motor	0.5	0.3	0.5	0.3	0.5	0.3	0.5	0.3	0.5	0.3	0.5	0.3				
Condenser	5.0	15.0	5.0	15.0	5.0	15.0	5.0	15.0	5.0	15.0	5.0	15.0				
Filter/separator	0.7	1.6	0.7	1.6	0.7	1.6	0.7	1.6	0.7	1.6	0.7	1.6				
By-product Valve	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1				
Water Valve	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1				
Piping/fittings	0.3	1.0	0.3	1.0	0.3	1.0	0.3	1.0	0.3	1.0	0.3	1.0				
Condenser for Exhaust	5.0	15.0	0.0	0.0	5.0	15.0	0.0	0.0	5.0	15.0	0.0	0.0				
Pump for exhaust water	0.3	0.3	0.0	0.0	0.3	0.3	0.0	0.0	0.3	0.3	0.0	0.0				
Subtotal	19.5	96.9	15.2	111.7	21.2	147.1	17.4	191.8	23.9	247.2	20.9	351.1				
Slurry			51.5				103.0				206.1					
Reaction Water to Carry			33.5				67.0				134.0					
Byproduct Water to Carry			0.0				0.0				0.0					
Byproduct		80.0			160.1				320.1							
Total	99.6	96.9	100.3	111.7	181.3	147.1	187.5	191.8	344.0	247.2	361.1	351.1				
<b>Stored Energy, kWhrth</b>	<b>166.6</b>				<b>166.6</b>				<b>333.1</b>				<b>666.3</b>			
<b>Specific Energy, kWh/kg, kWh/L</b>	<b>1.7</b>				<b>1.7</b>				<b>1.8</b>				<b>1.9</b>			