Proceedings of the 2000 DOE Hydrogen Program Review
NREL/CP-570-28890

Analysis of the

Sodium Hydride-based Hydrogen Storage System

being developed by

PowerBall Technologies, LLC

Prepared for

The US Department of Energy
Office of Power Technologies
Hydrogen Program

Prepared by

J. Philip DiPietro
and
Edward G. Skolnik,

Energetics, Incorporated

October 29, 1999

Analysis of the Sodium Hydride-Based Hydrogen Storage System being developed by PowerBall Technologies, LLC

We considered the viability of a system for storing hydrogen on-board a vehicle in the form of plastic-encapsulated sodium hydride (NaH) pellets. Hydrogen is produced when the pellets are cut and immersed in water. The exposed NaH surface reacts with water, releasing hydrogen and forming sodium hydroxide (NaOH) as a byproduct. Later, in an off-board activity, the hydroxide is recycled to hydride via a multi-step regeneration process that relies on methane as both a fuel and a reactant. This is a preliminary analysis that required the development of conceptual designs for several of the process steps and the need to make several assumptions in order to complete the overall systems analysis. The analysis was peer reviewed by several members of their hydrogen community, and their comments were taken into account in the preparation of this document.

Executive Summary

The reaction of sodium hydride with water to form hydrogen and sodium hydroxide can be utilized onboard a vehicle to deliver hydrogen to an onboard power system. PowerBall Technologies, LLC has developed a novel means of controlling the reaction: they encapsulate small amounts of sodium hydride in plastic balls. These balls are sliced open one at a time onboard the vehicle to deliver hydrogen as needed. We estimate a sodium hydride-based storage system can achieve a hydrogen storage density of 4.3 wt% and 47 kg/m^3, including all ancillary equipment. PowerBall Technologies, LLC is also developing a novel method of manufacturing the sodium hydride material. Instead of the traditional electrochemical process, they propose to form sodium metal by reacting natural gas and sodium hydroxide. A preliminary assessment indicates the cost of hydrogen delivered to a vehicle is about \$5.3/kg (\$39.4/MMBtu) using the sodium hydride system being developed by PowerBall Technologies, LLC. The implementation of cost reduction steps, based primarily on an alternative source of NaOH, results in a decrease of the cost of hydrogen to about \$4.1/kg (\$30.5/MMBtu).

One large component of the cost of the process is the energy requirements, with the key factor being the cost of regenerating the sodium hydride from sodium hydroxide. The full life-cycle energy consumption of the base case sodium hydride process is 4.0 kWh of energy per kWh of hydrogen delivered to the vehicle compared to 2.2 and 1.7 for liquid hydrogen and compressed hydrogen gas, respectively.

A comparison of the cost of delivered hydrogen from the PowerBall process with compressed hydrogen and liquid hydrogen is \$5.3/kg for the base case PowerBall process, \$4.1/kg for the lower cost PowerBall option, \$ 1.4/kg for compressed hydrogen, and \$2.8/kg for liquid hydrogen. When one includes the estimated cost of the respective on-board systems, however, the numbers become somewhat closer. The onboard equipment for the PowerBall process is estimated at about \$0.46/ kg H_2 compared to the capital cost of a pressure vessel, \$750, which equals about \$0.88/kg of hydrogen stored over the life of a vehicle. The overall costs are then about \$5.76/kg for the base-case PowerBall system, \$4.56/kg for the lower cost PowerBall system, \$2.28/kg for compressed hydrogen, and \$3.30/kg for the liquid hydrogen system.

A comparison can also be made between the cost of hydrogen from the PowerBall system, and the cost of gasoline. Using the comparative values of 31.4 miles/gallon gasoline for a standard AIV (Aluminum Intensive Vehicle) Sable, and 82.3 miles per gallon-equivalent for a fuel cell vehicle[1], a hydrogen cost of $5.30/kg is roughly equivalent to a gasoline cost of $2.02 per gallon, not including taxes. (An on-board hydrogen fuel cell vehicle will be more fuel-efficient than a gasoline ICE vehicle). A hydrogen cost of $4.10/kg is roughly equivalent to $1.56 per gallon (untaxed).

Aside from the relatively low cost of the on-board PowerBall operating system, another "plus" is the fact that the encapsulated ball system is amenable to the initial situation of a small number of vehicles in a geographic area.

It should also be pointed out that the application of the PowerBall technology in the chemical industry represents an attractive option. The estimated plant gate manufacturing cost of sodium metal via PowerBall Industries' thermochemical process could be as much as ten times less than the current commodity price for sodium produced via electrolysis. Also, the encapsulation concept could greatly lower the cost of transporting sodium and/or sodium hydride. PowerBall might consider pursuing applications for its technologies within the chemical industry in the near term, with a plan to expand into energy systems in the future.

Recently, PowerBall unveiled a modified recycling process. In this process, the syngas ($CO + H_2$) which is formed during the first step of the recycling process is in part combusted to produce heat to raise the reaction temperature, and in part reacted to produce more methane feedstock. As an addendum to this report, we have addressed this modification in the form of a very preliminary analysis.

PowerBall has indicated that the overall modified process is superior in that it produces more hydrogen per unit methane, and that the overall reaction is exothermic. Our preliminary analysis indicates that while

- *The amount of hydrogen produced per unit methane has indeed increased, and*
- *The overall reaction is exothermic.*

The following mitigating factors need to be considered as well:

- *The exothermicity of the overall reaction is in part due to the inclusion of a step (the hydriding of sodium) which is done separately, and from which the heat likely could not be used in the integrated process. Without this step, the overall reaction is endothermic.*
- *The benefit incurred by the decrease in the amount of methane feedstock needed is likely more than offset by the need for multiple separations, multiple reactors, and the added cost of oxygen to burn the syngas.*

---

[1] "Integrated Analysis of Hydrogen Passenger Vehicle Transportation Pathways", C.E. Thomas et al, Directed Technologies, Inc., Report to the National Renewable Energy Laboratory, Subcontract AXE-6-16685, March 1998.

Background

The PEM fuel cell has potential to be the next-generation vehicle power system, but delivering pure hydrogen fuel to the PEM stack, either through onboard storage of neat hydrogen or the processing of fossil fuels on-board, remains a barrier on the basis of cost, weight, and/or volume. The two commercially available options for onboard storage of hydrogen, compressed gas or liquid, are energy-intensive and would require significant investment in distribution infrastructure.

The Department of Energy's Hydrogen Program seeks to improve the commercial viability of hydrogen-based energy systems, and the Program is funding R&D into advanced hydrogen storage technologies, including chemical hydrides and carbon absorbents. Another approach being explored by PowerBall Technologies, LLC is to react a metal hydride with water to produce hydrogen gas and the corresponding metal hydroxide. Potential reactants include sodium, sodium hydride, calcium, and lithium. PowerBall Technologies, LLC has focused its efforts on sodium hydride because, compared to the others, it offers adequate weight and volume density, fast kinetics, and a clear recycle loop as will be discussed below.

The sodium hydride / water reaction {1} is strongly exothermic and proceeds vigorously upon contact of the reactants. In order to control the reaction for use as an onboard hydrogen source, PowerBall Technologies, LLC proposes that the sodium hydride be encapsulated in plastic-coated pellets (nominally 1.5 inches in diameter with a coating of polyethylene 0.020 inches thick). The pellets are stored onboard a vehicle, sliced open one at a time, and contacted with water to produce hydrogen as needed.

$$NaH + H_2O \dashrightarrow NaOH + H_2 \qquad -31.5 \text{ kcal/mole } H_2 \qquad \{1\}$$

The objective of this analysis is to characterize the sodium hydride-based hydrogen storage system and compare it to compressed gas and liquid hydrogen storage systems. The criteria for evaluation are:

1. Cost of hydrogen delivered to the vehicle
2. Weight and volume density of the onboard hydrogen storage system

Cost of Hydrogen Delivered to the Vehicle

The cost and fuel efficiency of the sodium hydride system is determined by an assessment of the production and delivery of sodium hydride balls to the vehicle. Sodium hydride is available as a specialty chemical, however its cost is prohibitive for use as a hydrogen carrier. The conventional process for sodium hydride manufacture, electrolyzing sodium chloride and then sparging hydrogen gas through a bath of the molten sodium metal, is too expensive for use as a hydrogen carrier. We can estimate the cost of the NaCl electrolysis process by considering the cost of product sodium. DuPont's list price for sodium metal is \$3.3/kg for bulk shipments (36,000 kg or more, http://www/dupont.com/sodium/price.mtml). Assuming it costs 20 cents/kg to produce sodium hydride from sodium metal by the sparging process, the estimated cost of sodium hydride is \$3.5/kg. Based on reaction {1}, twelve kg of NaH are required to deliver 1 kg of hydrogen gas. Thus \$3.5/kg of NaH converts to $42/kg ($300/MMBtu) of hydrogen delivered to the vehicle. Estimates of the cost of pressurized gas or liquid hydrogen delivered to a vehicle ranged from $1.4-2.8/kg. Clearly, the conventional process is too expensive.

The high cost of sodium hydride from the conventional production pathway is due to high-energy consumption. According to DuPont, the electrolysis of sodium chloride consumes 9.7 kWh of electricity per kg of sodium, which, based on reaction {1}, works out to 3.4 kWh electricity per kWh hydrogen delivered to a vehicle. When one considers that most U.S. electricity generation is fossil-based with an efficiency of 30% to 60%, the full life-cycle energy consumption of the sodium hydride system is even higher.

To achieve lower cost, PowerBall Technologies, LLC is developing a process for manufacturing sodium hydride from sodium hydroxide. Figure 1 is a schematic of the vehicle fueling system, in which vehicles consume sodium hydride balls and generate sodium hydroxide solution. At refueling stations, the sodium hydroxide solution is drained from the vehicles and replaced with a fresh load of sodium hydride balls. The hydroxide is stored at the vehicle refueling station and transported to a central facility where it is used as feedstock in the manufacture of new sodium hydride balls. The balls are then shipped out to the refueling stations to replenish their inventories.

Figure 2 is a block diagram of the process being developed by PowerBall Technologies, LLC for converting sodium hydroxide to sodium hydride. The process flow is as follows: 30 wt% sodium hydroxide is charged to a first stage concentrator where roughly 80% of the water is boiled off. Effluent sodium hydroxide solution (70 wt%) is charged to a second stage concentrator where the remaining water is boiled off, leaving molten sodium hydroxide (melting point of sodium hydroxide is 318 C). The molten sodium hydroxide is mixed with methane and charged to the sodium reactor, which is a molten bath of sodium carbonate (Na_2CO_3). The sodium carbonate serves to disperse the reactants and raise their temperature to roughly 980C. The following overall reaction occurs

$$NaOH + CH_4 \dashrightarrow Na + CO + 2.5\ H_2 \qquad +93.4\ \text{kcal/mole Na} \qquad \{2\}$$

The reactant products are gases and escape from the top of the reactor. The reaction is strongly endothermic, and heat must be supplied to the reactor by circulating a portion of the sodium carbonate bath through a heater vessel. The sodium carbonate is heated by burning a fuel and injecting the combustion exhaust into the bottom of the bath. The exhaust gases bubble up through the molten sodium carbonate bath, transferring heat. The transfer of sodium carbonate between the reactor and heater vessels is driven by the density difference of the hot and cold material. The sodium reactor heater fuel is preheated with exhaust gas effluent, and it is assumed that a 500C inlet temperature is achieved.

The effluent from the sodium reactor, CO, H_2, and Na at 980C, is quenched with Dowtherm or mineral oil, condensing the sodium at 880C at atmospheric pressure. The quench fluid is cooled by an air cooler.

Forty percent of the hydrogen contained in the quench overhead stream is recovered via a membrane or pressure swing absorber. The hydrogen is then bubbled up through the molten sodium product to produce sodium hydride. The carbon monoxide and hydrogen from the quench overheads (minus the hydrogen recovered for NaH production) is burned as fuel in the sodium reactor heater.

The concept is not entirely novel, as a United States patent was awarded to C. Netto of Germany in 1891 for the production of sodium from sodium hydroxide and carbon (patent number 460,985). In a patent filed in 1955 (patent number 2,930,689), McGriff moved the technology further. Among other ideas, he patented the concept of the sodium carbonate reactor.

Figure 2 contains a mass balance on the process based on 100 weight units of sodium hydroxide solution charged to the first stage concentrator (nominally kg/h). Also presented is the estimated duty of the heaters and coolers. The material balance is based on a process in which natural gas is used as both the carbon source for the sodium reactor and also to meet the process heating requirements.

Figure 3 shows a financial analysis of the NaH manufacturing process. We use a pro-forma cash flow model with capital, feedstock, and O&M costs as inputs. We then adjust the plant gate cost of sodium hydride to achieve an internal rate of return of 10% based on the after-tax cash flow.

The primary inputs into the financial analysis model are as follows:

> PowerBall Technologies, LLC estimates it will cost $1 million to build a pilot plant with a capacity of 45 kg/hr of sodium hydride production (unit cost $22,000/kg/hr). Energetics has reviewed the cost estimate based on the results of the heat and material balance. The pilot plant makes enough sodium hydride per year to supply power balls to roughly 250 passenger vehicles. Our financial analysis is based on a commercial unit that produces 450 kg/hr of sodium hydride with a unit cost of $10,000/kg/hr of NaH production capacity.
>
> The O&M cost is estimated to be 6% of capital. This rather high estimate is based on the corrosive nature of the materials involved leading to frequent parts replacement, and the high labor cost associated with ensuring safe operation.
>
> The natural gas consumption is 1.0 kg per kg of NaH production based on the material balance shown in Figure 2. The cost of natural gas is assumed to be $.42 /MMBtu ($.115 /kg, Annual Energy Outlook 1997 for industrial customers in the year 2000).
>
> We estimate that the sodium hydride balls will need to be transported via truck an average of 50 miles from the sodium hydride production plant to the dispensing stations. Also, the sodium hydroxide will be transported from the dispensing stations back to the sodium hydride production facility. We estimate the cost of truck transportation to be 10 cents per kg of hydrogen delivered to the vehicle.

The base case analysis gives a sodium hydride plant gate cost of $.44/kg which is substantially less than the cost derived from sodium chloride electrolysis of $3.8/kg. An NaH cost of $0.44 /kg translates to a delivered hydrogen cost of $5.3/kg. Table 1 shows that the natural gas feedstock represents 27% of the total sodium hydride manufacturing cost. As we have shown, the full life-cycle energy consumption of the base case sodium hydride process is high: 4.0 kWh of energy per kWh of hydrogen delivered to the vehicle (see addendum), compared to 2.2 and 1.7 for liquid hydrogen and compressed hydrogen gas, respectively. Notice that the truck transportation cost is a significant portion of the total cost.

Table 1. Cost break-down for NaH production

	cost $/kg NaH	Percent of total cost
Natural gas ($2.4/MMBtu)	0.12	27%
O&M (6% of capital)	0.08	17%
Capital recovery (10% IRR)	0.15	33%
Truck transportation	0.10	23%
Total	0.44	

Methods for Further Reducing the Sodium Hydride Production Cost

Figure 4 shows an alternative system in which spent sodium hydroxide from the vehicles is sold as a chemical feedstock and the sodium hydride manufacturing process is fed spent sodium hydroxide solution from industry. This process is considered feasible because 1) the spent sodium hydroxide from the vehicles should be relatively pure, and 2) the NaH production process being developed by PowerBall Technologies, LLC should be relatively tolerant of impurities and able to accept low-value spent sodium hydroxide solution. The system in Figure 4 will generate additional revenue due to the price differential between the caustic solution sold as a commodity chemical and the spent caustic taken from industry. The market price for sodium hydroxide solution ranges from 20 to 100 cents per kg. The developers would need to identify a spent industrial caustic that did not coke up the sodium hydroxide drying process. Also significant cost would be incurred in additional storage systems and in handling, marketing, and distributing the sodium hydroxide product. We estimate the net profits from such a system could equal 10 cents per kg of NaH ($1.20/kg of hydrogen).

Another method of reducing the natural gas cost would be to utilize by-product heat where possible. Table 2 shows the natural gas consumption broken out by its use in the process. Notice that the fuel credit from the syngas in stream 14 largely offsets the fuel required to provide the heat of reaction. By-product heat could be used instead of natural gas to concentrate the NaOH solution.

Another strategy for reducing costs is to substitute another hydrocarbon for natural gas. Because the natural gas charged to the sodium reactor is a carbon source for reaction {2}, the key criterion for displacing reactor feedstock is the cost per carbon atom. Table 3 shows the cost per carbon of several hydrocarbon feedstocks. No. 6 oil represents a 20% reduction compared to natural gas. Coal represents a 65% reduction in feedstock costs but would require increased capital for drying and solids handling equipment. Interestingly, diesel is more expensive per weight of carbon than natural gas.

Table 2. Natural gas consumption in the NaH production process

Stream number (from Figure 2)	Process use	Natural gas use	
		(kg CH4 / kg NaH)	percent of total
10	Fuel for concentrating the NaOH solution	0.32	21%
11	Reagent in the sodium reactor	0.64	42%
12	Fuel to provide heat of reaction	0.57	37%
	Subtotal	1.53	
14	Fuel credit from the by-product CO and H_2	-0.53	-35%
Total		1.0	

Table 3. Hydrocarbon cost, $/kg of carbon

Hydrocarbon	Cost	
	$/MMBtu*	$/kg carbon
Natural gas	2.42	0.154
Diesel	4.40	0.198
No. 6 Oil	2.55	0.114
Coal	1.48	0.050

* Annual Energy Outlook 1997, Industrial users 2000

Alternately, if a less expensive source of natural gas can be found, this also would lower the overall process cost. Personnel from PowerBall Technologies, LLC, have stated that stranded natural gas assets can be obtained for as little as $0.68/MMBtu, which is equivalent to $.043/kg carbon. This would lower the cost of NaH production from $0.44/kg NaH to $0.36/kg NaH. However, while this may open up applications in some areas, it is unlikely that this cost of natural gas could be maintained on a large-scale basis.

Table 4 compares the cost of liquid and compressed gaseous hydrogen estimated by Air Products and Chemicals in a study conducted with Directed Technologies for Ford Motor Company. The table shows that even under the aggressive low-cost scenario the sodium hydride system is more than twice as expensive as compressed hydrogen gas from a gas-station-sized steam methane reformer.

Table 4. Cost of delivered hydrogen from several onboard storage technologies		
	Cost of delivered hydrogen $/kg	Minimum number of vehicles served
Liquid hydrogen	2.8	400,000
Compressed gaseous hydrogen from a gas-station-sized steam methane reformer (100 factory built units)	1.4	1,000 per station, 100,000 total
Sodium hydride balls, base case	5.3	2,500
Sodium hydride balls, low cost case based on treatment of spent sodium hydroxide	4.1	2,500

The results from Table 4 should not discount the sodium hydride option. The liquid hydrogen cost is for a relatively large system. Small quantities of merchant, liquid hydrogen can be much more expensive, in the $5-7/kg range. With respect to gaseous hydrogen, in order to perform a comprehensive comparison, one must consider the cost of the onboard storage system. Table 5 shows the estimates for the cost of the onboard storage system for compressed gas, liquid hydrogen, and NaH systems. The sodium hydride system is inherently low-cost, and Table 5 shows that when levelized over the life of the vehicle, the cost of the onboard storage system per kg of hydrogen delivered to the power system is significant. This narrows the gap on the overall cost of using sodium hydride storage instead of compressed hydrogen: $4.76/kg for the NaH-based process (including profit from sale of NaOH) and $2.3/kg for compressed hydrogen. The cost for the liquid hydrogen system based on the same analysis is $3.3/kg.

Table 5. Onboard storage system cost analysis (systems with a storage capacity of 4 kg hydrogen)			
	Unit cost $/kg	Total cost $	Levelized cost $/kg H2 *
Compressed gas	190	760	0.88
Liquid hydrogen	100	400	0.46
Sodium hydride	100	400	0.46

*The capital recovery factor for the onboard hydrogen storage system equals 5.75 (based on an 8 year life and 8% interest rate). The levelized cost of the onboard storage system equals the annualized cost (initial cost / capital recovery factor) divided by the kg consumed by the vehicle per year. We assume a vehicle consumes 150 kg of hydrogen per year (80 miles per kg, 12,000 miles per year).

Energy Consumption in the Sodium Hydride-based Hydrogen Storage System

There are four sources of energy consumption associated with the sodium hydride system: 1) drying the sodium hydroxide, 2) raising the temperature of the system to 980C, 3) regenerating the hydride from the hydroxide, and 4) producing hydrogen from the hydride on-board. Table 6 below shows the various energy sinks in the sodium hydride-based hydrogen energy pathway.

By far the largest source of energy loss is in the conversion of sodium hydroxide to sodium hydride. Equation {2} below shows the primary conversion reaction.

$$NaOH + CH_4 \rightarrow Na + CO + 2.5\ H_2 \qquad \{2\}$$

The energy consumed by the conversion equals the heat value of the methane charge minus the heat value of the by-product carbon monoxide and hydrogen, plus the heat required to drive the reaction.

Energy required to convert NaOH to NAH	=	Heat value of stoichiometric methane	-	Heat value of by-product CO and H_2	+	Heat of Reaction, 93.4 kcal/mole

One mole of methane is consumed per each mole of sodium hydroxide reacted. Based on the heat of combustion of the natural gas consumed, 191.8 unit of heat energy are consumed per mole of sodium hydroxide reacted.

$$\frac{1\ \text{mole CH4}}{1\ \text{mole Na}} * \frac{191.8\ \text{kcal}}{\text{mole Ch4}} = 191.8\ \text{kcal heat / kcal NaOH reacted}$$

The heating value of by-product hydrogen and carbon monoxide is calculated as follows:

Hydrogen
$$\frac{2\ \text{mole}\ H_2}{\text{mole NaOH}} * \frac{28{,}700\ \text{kcal}}{\text{kg}\ H_2} * \frac{0.002\ \text{kg}\ H_2}{\text{mole}\ H_2} = 114.8\ \text{kcal / mole NaOH}$$

Carbon Monoxide
$$\frac{1.0\ \text{mole H2}}{\text{mole NaOH}} * \frac{2{,}415\ \text{kcal}}{\text{kg CO}} * \frac{0.028\ \text{kg CO}}{\text{mole CO}} = 67.6\ \text{kcal / mole NaOH}$$

Note that the amount of hydrogen is reduced from 2.5 moles to 2.0 moles to account for the hydrogen consumed in making NaH from Na:

$$Na + \tfrac{1}{2} H_2 \rightarrow NaH \qquad \{3\}$$

Table 6. Energy losses in the sodium hydride-based hydrogen energy pathway

Process stage	Heat lost, Btu of thermal energy per Btu of hydrogen energy delivered to the vehicle	Notes
Drying the sodium hydroxide solution*	0.44	Assume a two stage drying process; the first stage takes the solution from 50% to 75%, and the second takes it from 75% to 100%. Assume the steam from the second stage is re-condensed in the first stage.
Raising the temperature of the reactants to 980C	0.22	Assume 50% of the duty is achieved via heat integration
Conversion of sodium hydroxide to sodium hydride	2.81	Assume by-product CO and H2 are burned for heat value in an 80% efficient burner. Heat consumption includes the heat value of the methane consumed.
Conversion of sodium hydride to hydrogen fuel onboard	0.55	Exothermic reaction with water produces heat on-board the vehicle, which is dissipated.
Total	4.02	

Note that for this analysis we have assumed a 50 wt % solution as opposed to 30 wt % in the base case analysis contained in the report. This reduces the amount of water that must be boiled off per unit of sodium by a factor of 2, although the impact on the overall energy consumption is small.

To calculate the net energy requirement from the reactor we assume that the hydrogen and CO burner is 80% efficient, and also that the transfer of heat into the reactor vessel is 80% efficient. The energy consumed is thus:

$$191.8 + 93.4 / 0.8 - 0.8 * (114.8 + 67.6) = 162.6 \text{ kcal/mole NaOH reacted}$$

For each mole of sodium hydroxide, one mole of hydrogen is provided to the vehicle power system. Each mole of Na is converted to NaH using a portion of the byproduct hydrogen as shown in reaction {3}. Since the heat from this exothermic reaction is non-recoverable, it is not included in this calculation.

Next, the 162.6 kcal/mole NaOH must be expressed in a hydrogen-equivalent manner. Each mole of NaH provides one mole of hydrogen to the vehicle power system upon reaction with water as shown in reaction {1}.

$$NaH + H_2O \rightarrow NaOH + H_2 \qquad \{1\}$$

Based on a lower heating value of hydrogen of 57.8 kcal/mole, energy consumption is as follows.

$$\frac{162.6\text{ kcal}}{\text{mole NaOH}} * \frac{1\text{ mole NaOH}}{1\text{ mole H}_2} * \frac{1\text{ mole H}_2}{57.8\text{ kcal}} = 2.81\text{ kcal energy / kcal hydrogen}$$

The total energy consumed by the sodium hydride pathway, 4.02 kcal of energy per unit of hydrogen energy delivered, is high compared to liquid and pressurized gaseous storage (2.2 and 1.7 Btu energy per Btu of hydrogen delivered respectively). The estimate is credible when one considers that the overall steam methane reforming reaction as shown below produces four hydrogen molecules per methane molecule compared to only one hydrogen molecule per methane in the sodium hydride process.

$$CH_4 + H_2O \rightarrow CO_2 + 4\ H_2 \qquad \{4\}$$

Weight and volume density of the onboard hydrogen storage system

Weight density is defined as the kg of hydrogen fuel delivered to the on-board power system divided by the total weight of the hydrogen storage system, including ancillary equipment. Similarly, volume density is defined as the kg of hydrogen delivered to the vehicle per cubic meter of space that the hydrogen storage system takes up.

In order to develop a weight and volume density estimate, we characterized a sodium hydride-based hydrogen storage system designed to deliver 4.09 kg of hydrogen (a vehicle range requirement of 380 miles and a fuel efficiency of 93 miles per kg of hydrogen). Twelve kg of sodium hydride are required for each kg of hydrogen delivered to the PEM fuel cell, giving a total sodium hydride requirement of 49 kg.

PowerBall claims that they are able to compact NaH to a density of 1.1 g/cc. Thus, a 1.5-inch diameter ball would hold 0.0319 kg of NaH; 1,540 balls would be required to hold a total of 49 kg of NaH. At the peak rate of hydrogen consumption by the PEM fuel cell, the ball slicer will be cutting NaH balls at the rate of fourteen per minute to maintain hydrogen supply.

The onboard hydrogen storage system is shown in Figure 5 and works as follows: As the PEM fuel cell is operated it draws hydrogen gas from the storage system. A ball-slicing device retrieves a plastic-coated sodium hydride ball from the inventory and slices it open so that the sodium hydride is contacted with the water, producing hydrogen gas. The rate of ball slicing is controlled to maintain the pressure in the tank between 120 and 150 psi.

The ball slicing device developed by PowerBall Technologies, LLC works as follows. A ball is corralled into a cartridge tube. The cartridge is then closed and a burst of high-pressure hydrogen gas accelerates the ball through a blade assembly and into a water reservoir where the sodium hydride reacts to form hydrogen gas. The high-pressure hydrogen gas is produced by a small intensifier that takes 120 psi hydrogen gas from the main containment vessel and divides it into a high-pressure stream (250 psi) and a low-pressure stream (30 psi). The high-pressure stream is used by the ball slicer, and the low-pressure stream is discharged to a small buffer tank that feeds the PEM fuel cell. This is a somewhat complex system compared to an electric motor slicer, but it has the advantage that it does not represent a parasitic load and actually helps dissipate some of the thermal energy from the sodium hydride reaction.

Because the PEM fuel cell produces water as a by-product (the overall electrochemical reaction is shown below), it can supply the water required for the sodium hydride reaction, thus lowering the required weight of the system.

$$H_2 + \frac{1}{2} O_2 \text{ --> } H_2O + \text{electricity} \qquad \{5\}$$

Inspection of reactions {1} and {5} indicates that the fuel cell could provide all the water required by the sodium hydride system. However, practical considerations require extra water: 1) some of the water produced in the PEM fuel cell escapes in the wet exit gas; 2) a water inventory is needed for start-up; and 3) it is possible that sodium hydroxide, being hygroscopic, may become associated with reactant water, making some of the water unavailable for reaction (this issue requires further investigation; it could increase the system water requirement and/or necessitate on-board dehydration and segregation of the sodium hydroxide product). Thus, we assume the initial water inventory equals 50% of the stoichiometric requirement.

Because the reaction {1} is strongly exothermic, the storage system will likely heat up during vehicle operation. We estimate the sodium hydride storage system will increase the onboard cooling duty by 100% and increase the weight of the radiator system by 75%.

The containment vessel will consist of a plastic liner for corrosion resistance and a stainless steel or carbon/glass fiber shell to provide strength. If stainless steel is used, the weight of the vessel could be 30 kg. We have lowered the estimate of the containment vessel to 20 kg assuming advanced materials are used.

Table 7 shows the weight and volume of the components of the sodium hydride hydrogen storage system. The sodium hydride balls are the primary component, representing 56% of the weight and 51% of the volume. This indicates that significant weight and cost reductions below the estimates presented are unlikely to be achieved in real systems.

Interestingly, the storage system gets heavier as hydrogen is consumed. This is because water from the PEM fuel cell that would otherwise be discharged from the vehicle is reacted with sodium hydride and the oxygen atom is captured in the sodium hydroxide product. Assuming that 10% of the water content remains with the depleted system, we estimate the weight of a fully depleted tank to be 113.6 kg. This is an equivalent weight density of 3.6%.

Figure 6 shows that the sodium hydride system weighs more than compressed hydrogen gas and liquid hydrogen, but is more compact. That trade-off is similar to the one presented by magnesium hydride systems. The primary performance difference between the magnesium hydride systems and the sodium hydride/water system is that the magnesium system's hydrogen release reaction is endothermic (it uses waste heat from the onboard power system and/or burns a portion of the hydrogen parasitically), whereas the sodium hydride system generates a large amount of heat when it releases hydrogen. This means that the sodium hydride is simpler in that it does not have to be heat integrated with the on-board power system. On the other hand, because the heat generated onboard is lost, the sodium hydride system is inherently less energy-efficient.

Table 7. Estimated size and weight of a Power Ball system designed to deliver 4.1 kg of hydrogen to a vehicle power system

Component	Weight (kg)	Volume (m^3)
Sodium hydride balls	49	.0445
Water	18.4	.0184
Vapor space	Negligible	.0249
Container	20	negligible
Incremental radiator requirement	7	negligible
Ball slicer	3	negligible
Total	97.4	0.0879
Weight density	4.2%	
Volume density	46.6 kg/m^3	

The density analysis above assumes that the reaction of the cut sodium hydride pellets and water will be essentially stoichiometric. In fact, in the absence of mixing, the reaction will become diffusion limited, and consequently less efficient on a kinetic basis. As a result, excess water will need to be used to increase the reaction rate. At a reasonable value of 1.5 times stoichiometric for the amount of water needed, the weight density of the system is reduced to 3.8 % (3.3% based on a depleted tank), and the volume density is about 42.2 kg/m^3.

Other Concerns

Materials Concerns

Sodium hydride is regarded as an extremely reactive material and any system using it will come under close scrutiny for safety. Of concern is the potential for a chain reaction, in which the coating of one of the balls in the ball storage tank breaks for whatever reason (perhaps in a car crash) and reacts with water. The heat from this reaction then melts the coating of another balls and so on. A full safety analysis of the proposed on-board storage system is needed.

The density of NaH as claimed by PowerBall is 1.1 g/cc. This is the value we used above to calculate weight and volume system densities. Literature values for NaH, however, indicate that the density is actually 0.92 g/cc. With this lower density, the volume required for the PowerBalls would be about 16 % higher (including air space, 27% higher) than shown in Table 7.

Sodium hydroxide, though commonly used, is a caustic material and is hazardous. Siting of NaOH storage tanks in commercial areas where vehicle service stations are typically sited could cause resistance from local authorities. Also, onboard storage of sodium hydroxide solution will require Department of Transportation approval.

Above 30 wt%, aqueous solutions of sodium hydroxide freeze above 0 degrees Celsius. The NaH system must be designed to either avoid high concentration of sodium hydroxide to manage frozen reactant products.

Engineering/Processing Concerns

The storage system cost estimate may be low in that it does not include extensive coolant systems, buffer tanks, and interconnectivity. Nor is a method included for removal of the spent hydroxide liquid and refilling the tanks with water and PowerBalls. It has been hypothesized that the hydrogen-liberating reaction can be run stoichiometrically, leaving a dry hydroxide product, which would be easy to remove. Such a system would likely be difficult to control, especially due to the hygroscopic nature of NaOH.

The upcoming operation of the PowerBall Technologies, LLC pilot plant will be very instructive regarding the feasibility of sodium hydroxide-fed sodium hydride production. Anticipated issues include: corrosion of the submerged heater, coking in the sodium hydroxide dryer, temperature controls in the reactor, recovering heat from the sodium reactor heater, and recovering hydrogen from the reactor off-gas. A more detailed process cost estimate should be completed after the benefits of the pilot plant operation are available.

If the operating pressure of the onboard storage system were raised, it would be possible to power the PEM fuel cell air compressor via a hydrogen-fed expansion turbine. In addition to reducing the parasitic electric load of the air compressor, the expander would reduce the cooling requirements. This concept has been investigated for pressure vessel systems. It was largely abandoned because of cost and also because the pressure is gradually reducing as the tank is emptied. In the sodium hydride system, the pressure can be controlled over the full storage cycle by varying the rate of ball slicing. However, a high-pressure system would require a heavier containment tank. The trade-offs associated with this concept should be investigated in more detail.

Garnering additional revenues by supplying the sodium hydride production process with spent industrial caustic solution can substantially reduce the cost of sodium hydride. In many cases spent industrial caustic solutions fall under environmental regulations. Such regulations could affect handling requirements of the feedstock and the solids from the bottom of the sodium reactor and heater. Such regulations, if applicable, could diminish the economic incentives. A set of environmental case studies could be useful to assess the feasibility of this concept.

Environmental Concerns

Aside from the environmental concerns voiced above, dealing with the handling of NaOH, there is the question of CO_2 emissions. The regeneration reaction (reaction (2)) is powered by burning methane, CO and hydrogen, resulting in the formation of CO_2. The amount of CO_2 produced is likely greater than current gasoline engines given the 4 to 1 energy requirement to deliver hydrogen. On the other hand, CO_2 production in the PowerBall case would be centralized, and therefore amenable to sequestration options. Overall CO_2 to the atmosphere would therefore likely be less. At any rate, if the PowerBall option is to be viable, greenhouse gas effects need to be given a closer look.

Conclusions

The base case cost of the sodium hydride system corresponds to a cost of hydrogen delivered to the vehicle power system of $5.30/kg. A low-cost scenario reduces this cost to $4.10/kg. The low-cost case is twice as expensive than costs predicted for compressed hydrogen gas systems. However, the fact that the sodium hydride system is amenable to geographically dispersed hydrogen vehicles, and that it promises a relatively low-cost on-board storage system, may make it attractive. Including the on-board equipment, the low-cost case of the PowerBall system is a little over $1/kg more expensive than a comparable liquid hydrogen system, and a little over $2/kg H_2 more expensive than a compressed hydrogen system. The safety features and ease of transportation of the encapsulated NaH pellets increases the attractiveness of the system, making it of interest at least to niche markets.

An onboard hydrogen storage system using plastic-coated balls of sodium hydride may achieve a hydrogen storage density of 4.3 wt% and 47 kg/m^3 including all ancillary equipment. This is heavier, but more compact than compressed gas and liquid hydrogen systems.

Figure 1. Schematic Of The Sodium Hydride-based Hydrogen Storage And Delivery System

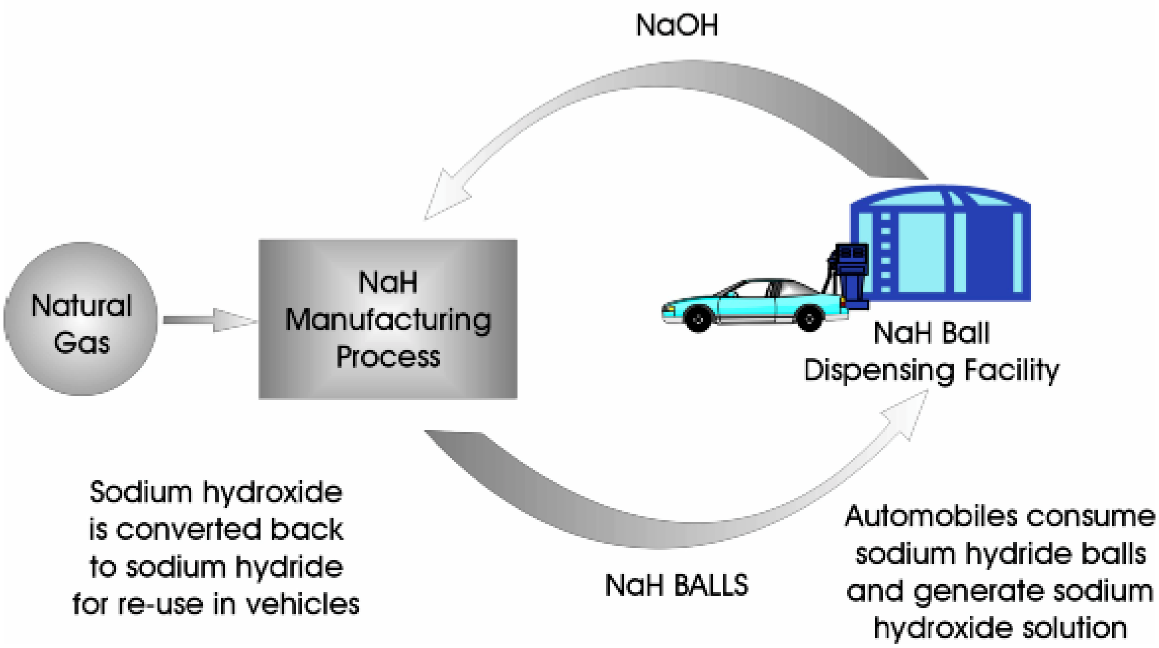
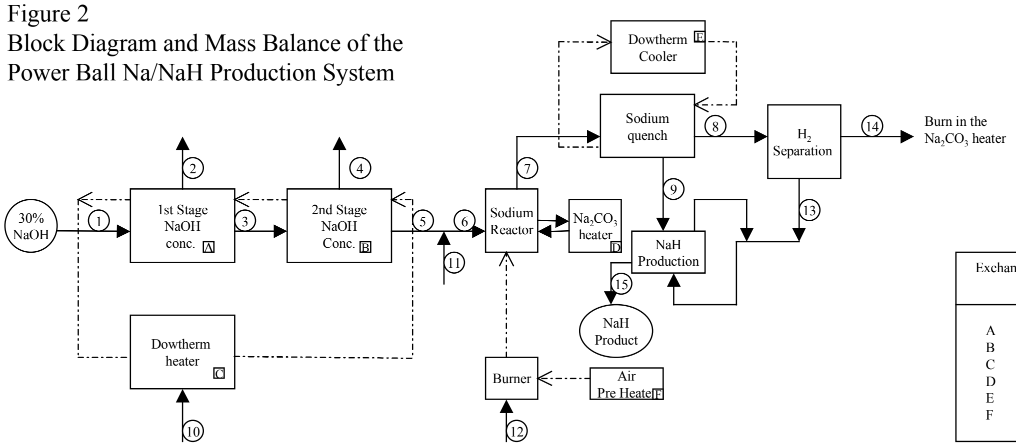


Figure 2
Block Diagram and Mass Balance of the
Power Ball Na/NaH Production System



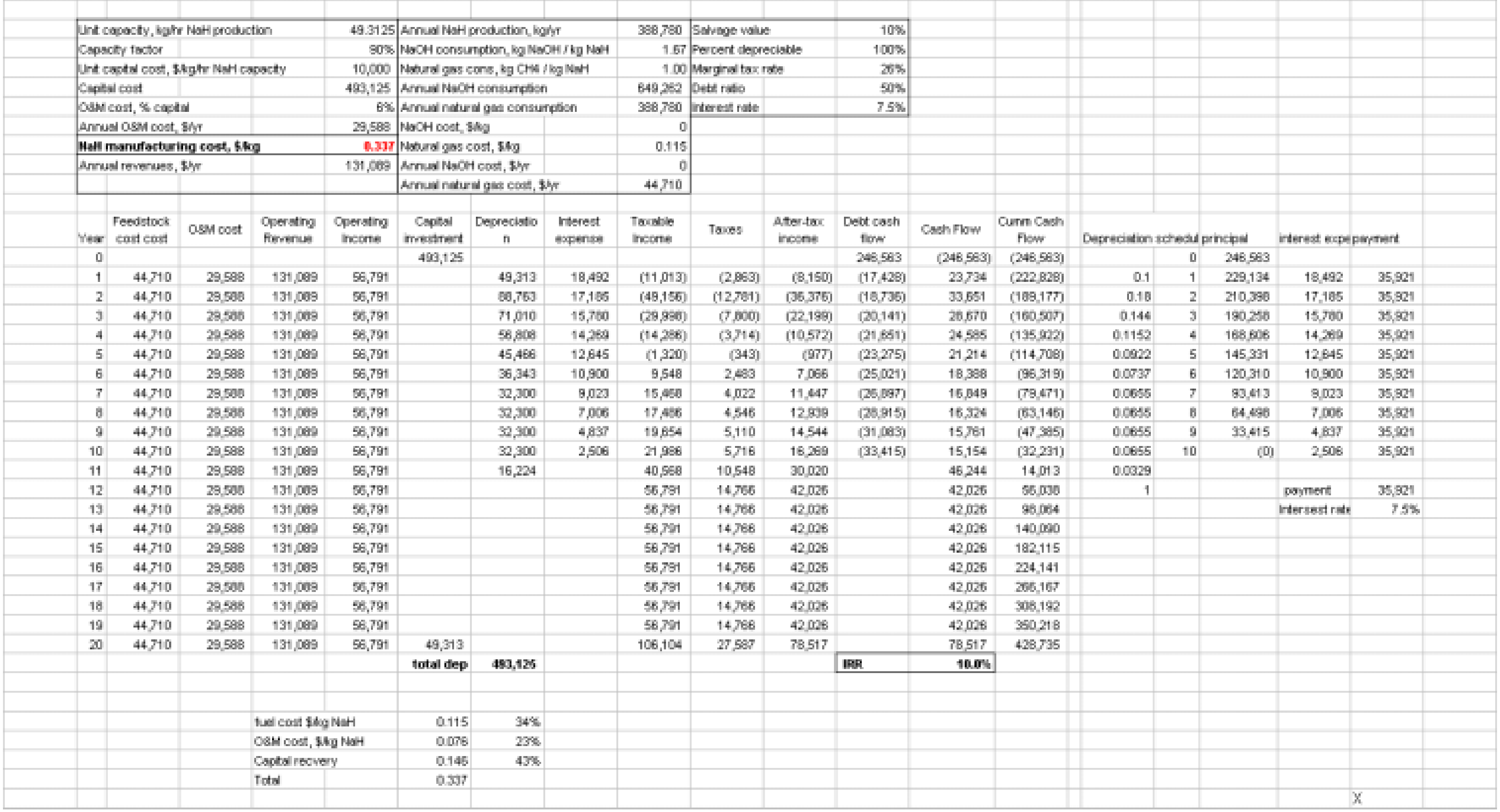
Exchanger	Duty kcal/h
A	33,500
B	16,500
C	59,000
D	88,000
E	23,000
F	16,189

—— Mass flow
-·-·- Heat flow

Flow Rates in kg/h

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
NaOH	30		30		30	30									
Na							17.25		17.25						
NaH															18.75
C															
CO							21.0	21.0						21.0	
H_2O	70	57	13	13											
CH_4						12				5.9	12	0.6			
H_2							3.75	3.75					1.5	2.25	
Total	100	57	43	13	30	42	42	24.75	17.25	4.9	12	0.6	1.5	23.25	18.75
Temp ^{0}C	20	120	120	320	320	320	980	500	500	20	20	20	300	300	

Figure 3. Analysis of PowerBall’s Sodium-Based Hydrogen Storage Concept, Cash Flow from NaH Production



Unit capacity, kg/hr NaH production	49.3125	Annual NaH production, kg/yr	388,780	Salvage value	10%
Capacity factor	90%	NaOH consumption, kg NaOH / kg NaH	1.67	Percent depreciable	100%
Unit capital cost, $/kg/hr NaH capacity	10,000	Natural gas cons, kg CH4 / kg NaH	1.00	Marginal tax rate	26%
Capital cost	493,125	Annual NaOH consumption	649,262	Debt ratio	50%
O&M cost, % capital	6%	Annual natural gas consumption	388,780	Interest rate	7.5%
Annual O&M cost, $/yr	29,588	NaOH cost, $/kg	0		
NaH manufacturing cost, $/kg	**0.337**	Natural gas cost, $/kg	0.115		
Annual revenues, $/yr	131,089	Annual NaOH cost, $/yr	0		
		Annual natural gas cost, $/yr	44,710		

Year	Feedstock cost cost	O&M cost	Operating Revenue	Operating Income	Capital investment	Depreciation	Interest expense	Taxable Income	Taxes	After-tax income	Debt cash flow	Cash Flow	Cumm Cash Flow	Depreciation schedul		principal	interest expe	payment
0					493,125						246,563	(246,563)	(246,563)		0	246,563		
1	44,710	29,588	131,089	56,791		49,313	18,492	(11,013)	(2,863)	(8,150)	(17,428)	23,734	(222,828)	0.1	1	229,134	18,492	35,921
2	44,710	29,588	131,089	56,791		88,763	17,186	(49,156)	(12,781)	(36,376)	(18,736)	33,651	(189,177)	0.18	2	210,398	17,185	35,921
3	44,710	29,588	131,089	56,791		71,010	15,780	(29,998)	(7,800)	(22,199)	(20,141)	28,670	(160,507)	0.144	3	190,258	15,780	35,921
4	44,710	29,588	131,089	56,791		56,808	14,269	(14,286)	(3,714)	(10,572)	(21,651)	24,585	(135,922)	0.1152	4	168,606	14,269	35,921
5	44,710	29,588	131,089	56,791		45,466	12,645	(1,320)	(343)	(977)	(23,275)	21,214	(114,708)	0.0922	5	145,331	12,645	35,921
6	44,710	29,588	131,089	56,791		36,343	10,900	9,548	2,483	7,066	(25,021)	18,388	(96,319)	0.0737	6	120,310	10,900	35,921
7	44,710	29,588	131,089	56,791		32,300	9,023	15,468	4,022	11,447	(26,897)	16,849	(79,471)	0.0655	7	93,413	9,023	35,921
8	44,710	29,588	131,089	56,791		32,300	7,006	17,486	4,546	12,939	(28,915)	16,324	(63,146)	0.0655	8	64,498	7,006	35,921
9	44,710	29,588	131,089	56,791		32,300	4,837	19,654	5,110	14,544	(31,083)	15,761	(47,385)	0.0655	9	33,415	4,837	35,921
10	44,710	29,588	131,089	56,791		32,300	2,506	21,986	5,716	16,269	(33,415)	15,154	(32,231)	0.0655	10	(0)	2,506	35,921
11	44,710	29,588	131,089	56,791		16,224		40,568	10,548	30,020		46,244	14,013	0.0329				
12	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	56,038	1			payment	35,921
13	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	98,064				Intersest rate	7.5%
14	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	140,090					
15	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	182,115					
16	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	224,141					
17	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	266,167					
18	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	308,192					
19	44,710	29,588	131,089	56,791				56,791	14,766	42,026		42,026	350,218					
20	44,710	29,588	131,089	56,791	49,313			106,104	27,587	78,517		78,517	428,735					
					total dep	**493,125**					**IRR**	**10.0%**						

fuel cost $/kg NaH	0.115	34%
O&M cost, $/kg NaH	0.076	23%
Capital recovery	0.146	43%
Total	0.337	

X

Figure 4. Potentially Higher Value System that also Provides Management of Spent Sodium Hydroxide Solution from Industry

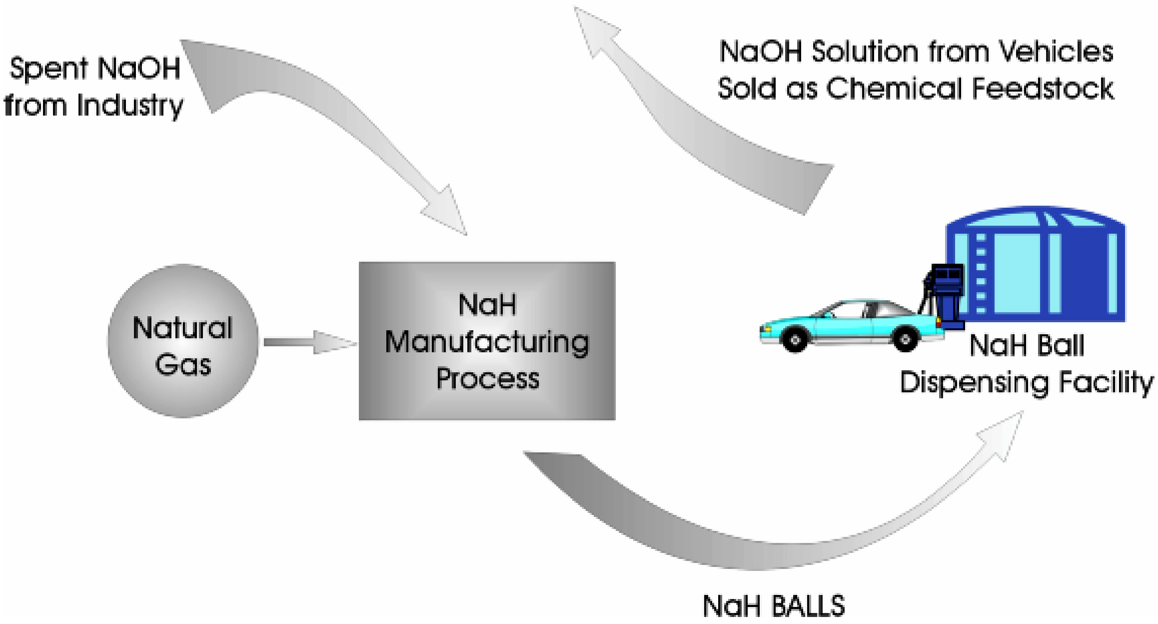


Figure 5. Schematic of a PEM Fuel Cell/Power Ball Hydrogen Storage On-board Power System

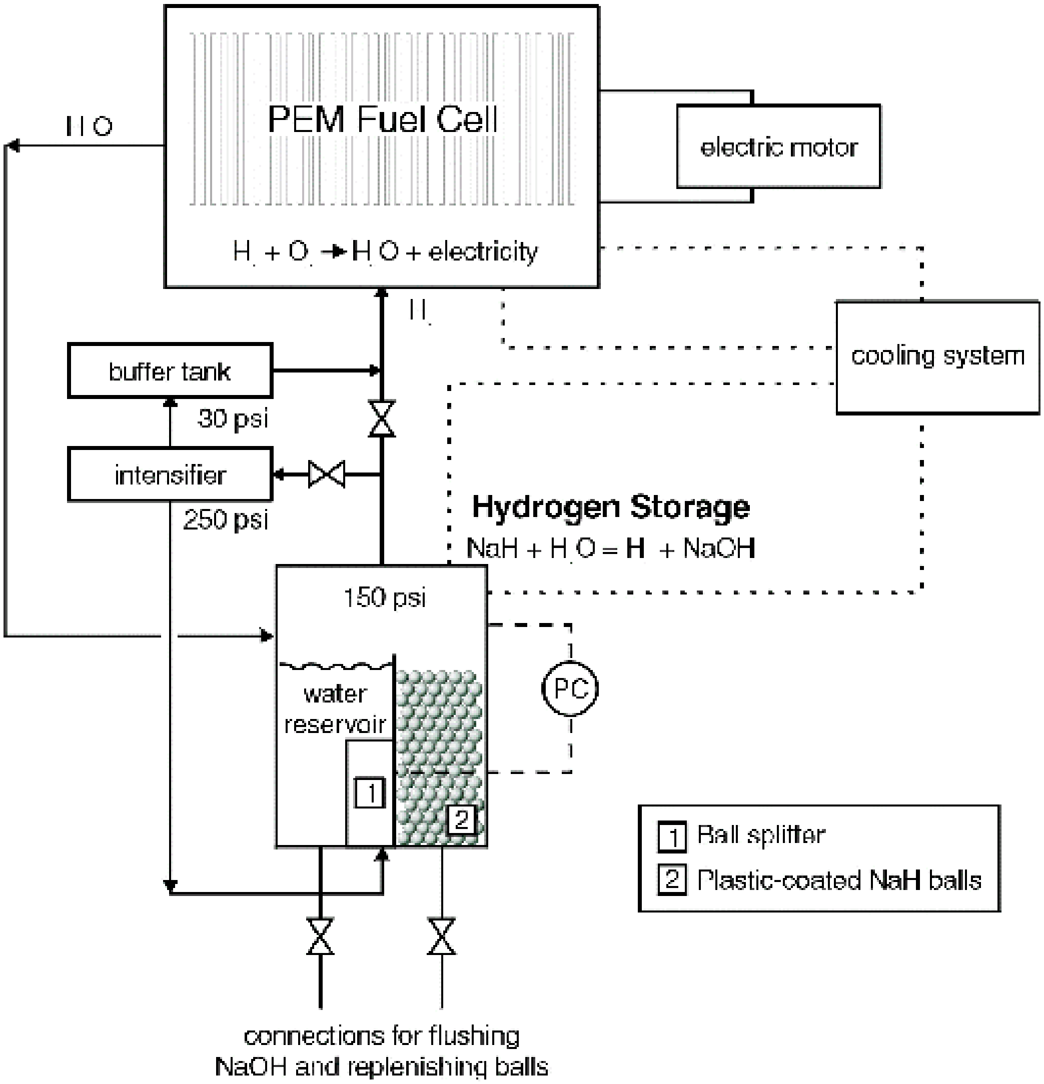
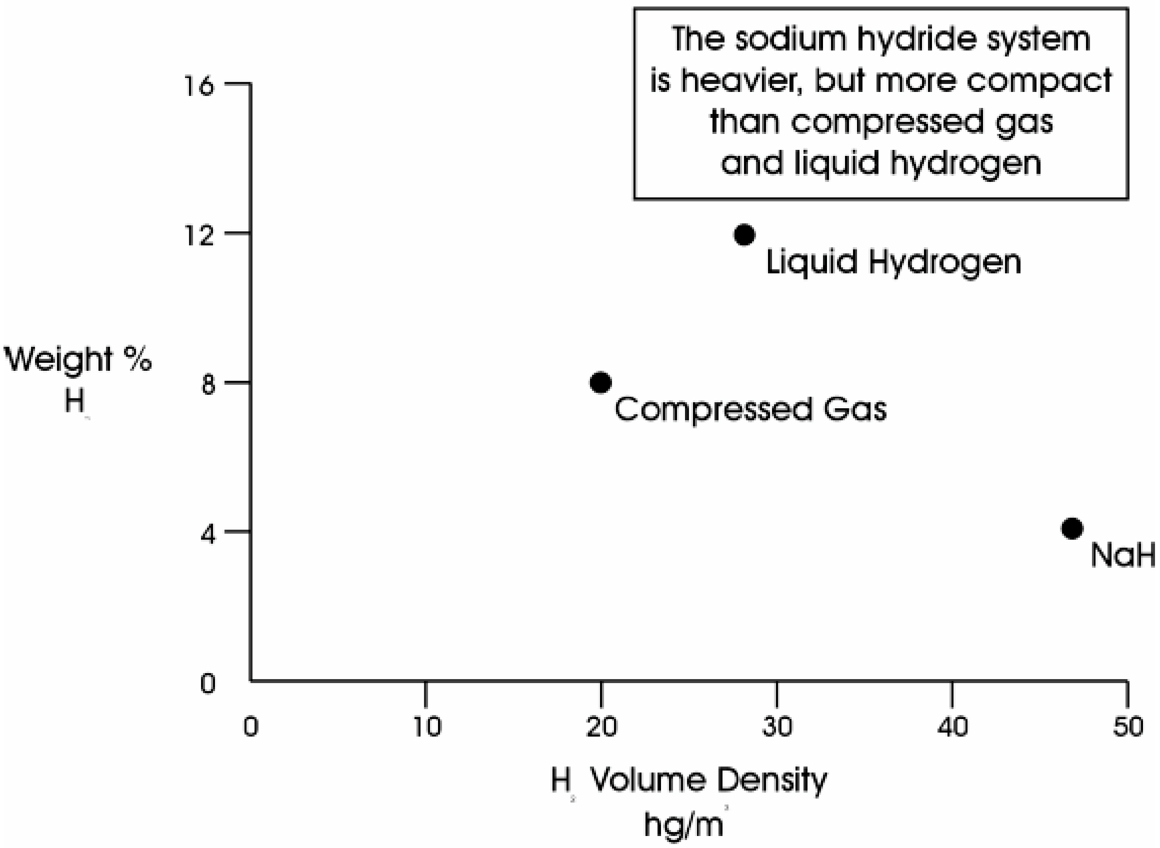


Figure 6. Hydrogen Storage Density*



* Based On Systems That Store 4.1 Kg Of Hydrogen

Addendum: Addressing A Change to the PowerBall Process

Note: To avoid confusion, we are continuing with the equation numbering scheme that was used in the main report.

PowerBall, Inc. has recently proposed a change to their overall schematic for producing and recycling their sodium hydride pellets. In their new scenario, they indicate that the overall reaction for the recycling process will be:

$$2\ NaOH + CH_4 + O_2 \rightarrow 2\ NaH + CO_2 + 2\ H_2O \qquad \{6\}$$

If this is combined with the on-board hydrogen-generation reaction:

$$2\ NaH + 2\ H_2O \rightarrow 2\ H_2 + 2\ NaOH \qquad \{1'\}$$

the result is:

$$CH_4 + O_2 \rightarrow 2\ H_2 + CO_2 \qquad \{1' + 6\}$$

So that in effect one mole of methane is being used to produce two moles of hydrogen.

PowerBall has indicated that a key factor in determining the viability of the recycling process that is being discussed here is the question of whether reaction {6} is exothermic. Reaction {6} is indeed exothermic, releasing 15.8 kcal/mole of methane.

However, some discussion is necessary as to the importance of this exothermicity. Reaction {6} is the result of a series of reactions and processes that involve the transfer of heat and mass, and thus any rational analysis must be based on a calculation that takes each of the individual component reactions into account. According to information supplied by PowerBall, the reaction would be carried out by first reacting methane with sodium hydroxide as in the previous scheme:

$$NaOH + CH_4 \rightarrow Na + CO + 2.5\ H_2 \qquad \{2\}$$

½ mole of hydrogen would still react with the sodium:

$$Na + 0.5\ H_2 \rightarrow NaH \qquad \{3\}$$

This leaves 2 moles of hydrogen and one mole of CO – a "syngas" mixture.

PowerBall then claims that about one half of the syngas can be combusted to provide the heat to run reaction {2}.

In order to provide the correct stoichiometry, we will use half of the CO, but only 0.5 mole of hydrogen:

$$0.5\ CO + 0.5\ H_2 + 0.5\ O_2 \rightarrow 0.5\ CO_2 + 0.5\ H_2O \qquad \{7\}$$

The remainder of the syngas, ½ mole of CO and 3/2 mole of hydrogen could then produce methane and water in the "reverse reforming" mode:

$$0.5\ CO + 1.5\ H_2 \rightarrow 0.5\ CH_4 + 0.5\ H_2O \qquad \{8\}$$

The methane product of reaction {8} can then be recycled to reaction {2}, etc. Thus, each subsequent recycling reclaims ½, ¼, 1/8, 1/16, etc. moles of CH_4 for further reaction.

As the recycling continues, the theoretical limits to equations {2}, {3}, {7}, and {8} become:

$$2\ NaOH + 2\ CH_4 \rightarrow 2\ Na + 2\ CO + 5\ H_2 \qquad \{2'\}$$

$$2\ Na + H_2 \rightarrow 2\ NaH \qquad \{3'\}$$

$$CO + H_2 + O_2 \rightarrow CO_2 + H_2O \quad \{7'\}$$

$$CO + 3\ H_2 \rightarrow CH_4 + H_2O \qquad \{8'\}$$

which combine to produce:

$$2\ NaOH + CH_4 + O_2 \rightarrow 2\ NaH + CO_2 + 2\ H_2O \qquad \{6\}$$

Thus, stoichiometrically, it is true as PowerBall has contended, that one mole (16 grams) of methane will produce two moles (48 grams) of sodium hydride, which will in turn lead to the on-board production of two moles (4 grams) of hydrogen:

$$2\ NaH + 2\ H_2O \rightarrow 2\ H_2 + 2\ NaOH \qquad \{1'\}$$

However, the overall exothermicity of equation {6} of –15.8 kcal, includes reaction {3'} as one of its components. This reaction occurs separately from the main recycling system, and its released heat cannot be used to aid in the recycle process. The reaction is exothermic by 28 kcal. Thus, the recycle process, which is composed of reactions {2}, {7'}, and {8'} combine as follows:

$$2\ NaOH + CH_4 + O_2 \rightarrow 2\ Na + H_2 + CO_2 + 2\ H_2O \quad \{9\}$$

is actually <u>endothermic</u> by 12.2 kcal in total, or by 12.2/2 = 6.1 kcal/mole of NaOH reacted

Even more important is the fact that in order to follow the recycling process scheme as described by PowerBall, and shown here by reactions {2}, {3}, {7}, and {8}, the reaction {2} products must be followed by separation into 4 product streams:

$$Na + CO + 2.5\ H_2 \rightarrow \begin{array}{l} Na \\ 0.5\ H_2 \\ 0.5\ CO + 0.5\ H_2 \\ 0.5\ CO + 1.5\ H_2 \end{array}$$

with the first and second streams reacted to regenerate the sodium hydride by reaction {3},
the third stream reacted to liberate energy for recycling in the system by reaction {7}, and the fourth stream reacted to form methane by reaction {8}.

It should be further pointed out that yet another separation is then necessary – the methane produced in reaction {8} must be separated from the water before being reintroduced into reaction {2}.

Reaction {2} must be run a high temperature to produce the desired products. This is evident from Figure A, which shows the major species that occur in equilibrium between an equimolar mixture of liquid NaOH and CH_4. To form sodium, the reaction is best run at a temperature greater than 1200 K (927 C) and preferably closer to 1300 K (1027 C). In order to separate sodium from this mixture, the gases must be irreversibly quenched to a low temperature, thus freezing the high temperature mixture composition. The quenching of the products has some energy loss associated with it. In addition, although the conversion of sodium is high, it is not 100%, and thus there will be some loss of sodium in this process.

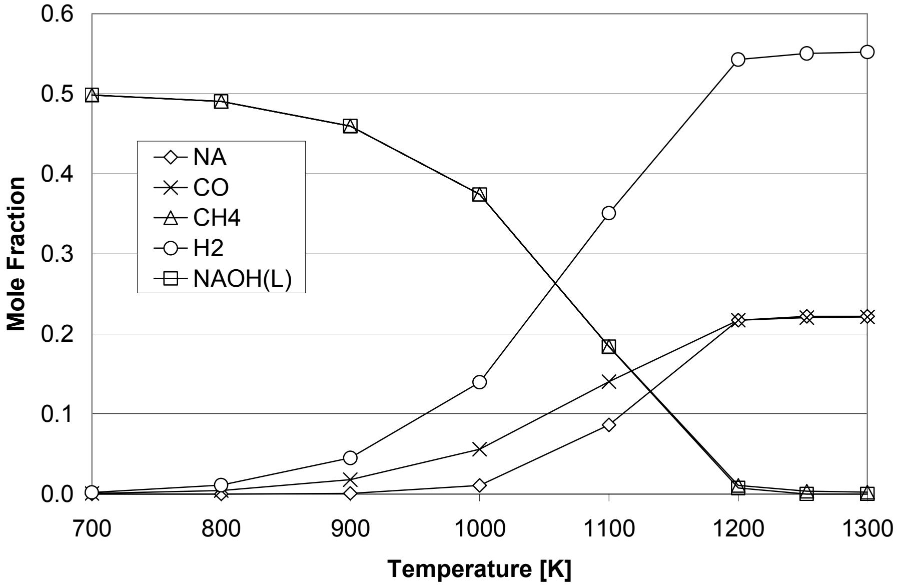


Figure A. Equilibrium composition of an equimolar mixture of methane and sodium hydroxide ($CH_4 + NaOH_{(L)}$)

Another form of loss that will occur is the energy expenditure and less that unity conversion efficiency from each of the 5 separation processes described above.

We can now repeat the analysis for energy consumption that was presented in the main body of the report, modified based on the new set of equations:

We note that the energy consumed by the conversion now equals the heat value of the methane charge plus the heat required to drive the reaction. The heating value of the syngas is now incorporated into the equation (equation {9}). Note, however, that there is now more Na produced per unit methane.

One mole of methane is consumed for every two moles of sodium hydroxide reacted. Based on the heat of combustion of the natural gas consumed, 191.8 unit of heat energy are consumed for every two moles of sodium hydroxide reacted.

$$\frac{1 \text{ mole } CH_4}{2 \text{ mole Na}} * \frac{191.8 \text{ kcal}}{\text{mole } CH_4} = 95.9 \text{ kcal heat / kcal NaOH reacted}$$

This is the heating value of stoichiometric methane, and is added to the heat of reaction {9}, 6.1 kcal/kcal NaOH reacted:

= 102.0 kcal/mole NaOH reacted. This is substantially lower than the energy requirement (162.6 kcal) for the original process.

On a hydrogen basis, as before, the energy requirement on a per hydrogen unit energy basis is calculated using the lower heating value of hydrogen:

$$\frac{102.0 \text{ kcal}}{\text{mole NaOH}} * \frac{1 \text{ mole NaOH}}{1 \text{ mole } H_2} * \frac{1 \text{ mole } H_2}{57.8 \text{ kcal}} = 1.76 \text{ kcal energy input / kcal hydrogen.}$$

We could also consider using the heat generated during the hydride production process,

$$Na + 0.5\, H_2 \rightarrow NaH \qquad \{3\},$$

-14 kcal/mole Na , as a drying source for NaOH. Recall that Table 6 showed the need of 0.44 energy units per energy unit of hydrogen produced to dry the hydroxide. Since each mole of Na eventually converts to one mole of hydrogen, the production of 57.8 kcal of hydrogen is preceded by the production of 14 kcal of heat during the hydriding step. Thus, there is a gain of 14/57.4 = 0.24 energy units/ energy units of hydrogen produced due to the hydriding step. If we assume an 80% heat transfer, this is still 0.19 units. This reduces the need of fuel to 0.44 – 0.19 = 0.25 units for this step.

In trying to look at the cost of the revised process, we must consider the fact that we have dropped the sodium carbonate heater and added what might be at first considered a more direct heating mechanism. However, due to the batch nature of the process, we are actually dealing with a different indirect heater – the walls of the reactor. We are also faced with the need either for a larger reactor to accommodate air as an oxygen supply, or to purchase reactant oxygen. Finally, we need a separate reactor to perform the reverse reforming reaction.

We can then modify Table 6 to incorporate these changes.

Table 6’. Energy losses in the sodium hydride-based hydrogen energy pathway

Process stage	Heat lost, Btu of thermal energy per Btu of hydrogen energy delivered to the vehicle	Notes
Drying the sodium hydroxide solution*	0.25	Assume a two stage drying process; the first stage takes the solution from 50% to 75%, and the second takes it from 75% to 100%. Assume the steam from the second stage is re-condensed in the first stage.
Raising the temperature of the reactants to 980C	0.22	Assume 50% of the duty is achieved via heat integration
Conversion of sodium hydroxide to sodium hydride	1.76	Includes the heating value of the methane used
Conversion of sodium hydride to hydrogen fuel onboard	0.55	Exothermic reaction with water produces heat on-board the vehicle, which is dissipated.
Total	2.78	

Note that for this analysis we have assumed a 50 wt % solution as opposed to 30 wt % in the base case analysis contained in the report. This reduces the amount of water that must be boiled off per unit of sodium by a factor of 2, although the impact on the overall energy consumption is small.

In addition, as already pointed out, the new process requires an increase in the number of separations necessary to provide reaction materials. In addition to the separation of sodium (already a factor in the original scheme) the separation of reaction {2} syngas components into three fractions would also be required. This would be manifested as 1) one-fifth of the H_2 for hydriding the sodium (as in the original system), 2) one-fifth of the H_2 and half of the CO to be combusted to provide heat, and 3) three-fifths of the H_2 and the other half of the CO to convert to methane. The separation of product methane from water represents yet another process. Membrane systems and pressure regulators could likely be set up to approximate this type of separation, but performing this inexpensively and efficiently represents a challenge to the project.

The improved utilization of methane as depicted by this revised process is offset by the additional expenses that are likely to be incurred by:

- The need for a separation process to provide the proper stoichiometry for the syngas combustion and the methane regenerating reactions,
- Either the need for a bigger reactor to accommodate air to oxidize the syngas, or the increased operating expenses that will be incurred to supply oxygen for the same process,
- The greater losses of efficiencies that come with more complex processes,
- The additional reactor needed to regenerate methane.

Disclaimers

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product or process disclosed or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government, or any agency thereof.

This research report was prepared by Energetics, Incorporated as an account of work sponsored by the United States Department of Energy, Office of Energy Efficiency and Renewable Energy Under Cooperative Agreement Number DE-FC36-98GO10291. Because of the nature of the work performed, neither Energetics, Incorporated nor any of its employees makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by Energetics, Incorporated.