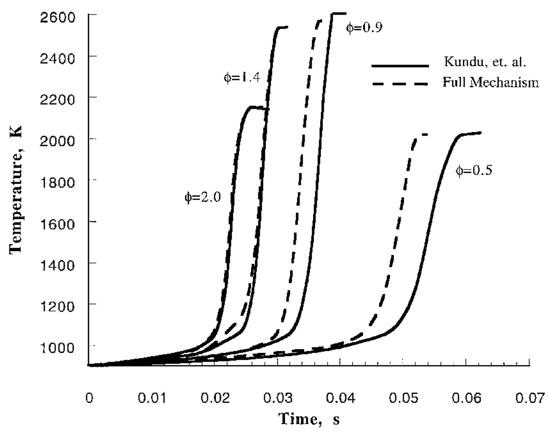

Fig. 3 Comparison of present mechanism with original mechanism for Jet-A reaction at four different equivalence ratios, for 1 atm and 1000 K initial conditions.

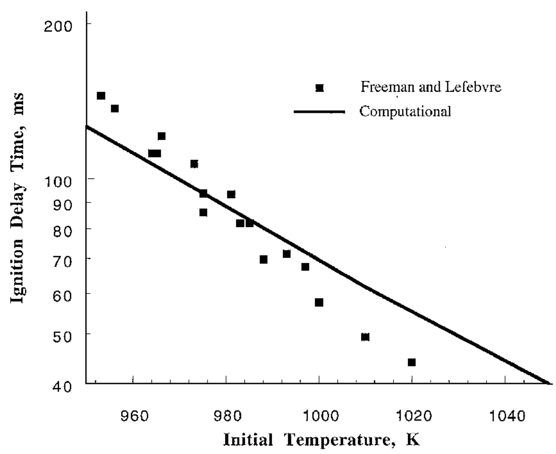

Fig. 4 Comparison of ignition delay time for Jet-A fuel at $\phi = 0.5$, 1 atm measured by Freeman and Lefebvre,[9] and the computational reaction mechanism, as a function of initial temperature.

the comparison of the present reaction mechanism and the original Jet-A mechanism. There is at most a 10% difference in the ignition delay time and a 5% difference in the final temperature between the present mechanism and the original. The present mechanism has also been matched to experimental data sets; each of the individual mechanisms cited has itself been validated, and the overall ignition delay time from the combined set has been compared to the data of Freeman and Lefebvre,[11] as shown in Fig. 4. Note that differences between the calculated ignition delay and experimental results are likely due to inconsistencies in defining that parameter: The experimental determination was done by visually locating a sudden pressure rise, whereas the computational result was set by a 20% temperature rise.[12]

Conclusions

A joint Jet-A/silane/hydrogen reaction mechanism has been constructed from existing mechanisms for modeling the combustion of Jet-A with silane as a pilot igniter. This model can now be used for studies of hydrocarbon combustor length and reaction efficiency, as a guide for design tradeoffs, and for experimental studies. For instance, a quasi-one-dimensional scramjet combustor model was implemented that included this present mechanism, from which it was shown that the addition of silane is indeed beneficial in decreasing the combustor length in a scramjet engine (though depending on the added fraction, specific impulse can suffer because of the reduced average heat of reaction).[12] At 1 atm, 1000 K, the characteristic reaction lengths for a hydrocarbon scramjet with 0.5 equivalence ratio and Mach 3 entrance conditions can be reduced from approximately 100 m with no piloting to 0.1 m with 20% silane addition. With 10% silane, the characteristic reaction length is approximately 1.2 m. However, the effective specific impulse for that combustor (calculated from the difference between maximum available thrust and total vehicle drag) will drop from 550 s without silane to 400 s with 10% silane and to less than 300 s with 20% silane.

References

[1] Lewis, M., and Gupta, A., "Impact of Fuel Selection on Hypersonic Vehicle Optimization," International Society for Air Breathing Engines, Paper 97-7200, Sept. 1997.

[2] Edwards, T., "Combustion Challenges of High Temperature Jet Fuels," American Inst. of Chemical Engineers, AIChE Annual Meeting, Chicago, IL, Paper 204a, Nov. 1996.

[3] Jachimowski, C. J., "An Analytical Study of the Hydrogen–Air Reaction with Application to Scramjet Combustion," NASA TP-2791, Feb. 1988.

[4] McLain, A. G., Jachimowski, C. J., and Rogers, R. C., "Ignition of Mixtures of SiH_4, CH_4, O_2, and Ar or N_2 Behind Reflected Shock Waves," NASA TP-2415, April 1985.

[5] Kundu, K. P., Penko, P. F., and Yang, S. L., "Reduced Reaction Mechanisms for Numerical Calculations in Combustion of Hydrocarbon Fuels," AIAA Paper 98-0803, Jan. 1998.

[6] Maurice, L. Q., "Detailed Chemical Kinetic Models for Aviation Fuels," Ph.D. Thesis, Univ. of London, London, Oct. 1996.

[7] Kee, R. J., Rupley, F. M., and Miller, J. A., "Chemkin-II: A Fortran Chemical Kinetics Package for the Analysis of Gas Phase Chemical Kinetics," SAND89-8009B, Sandia National Labs., Albuquerque, NM, April 1989, URL: http://www.nist.gov/cstl/div836/ckmech.

[8] "VODPK Routine," Netlib Repository, URL: http://www.netlib.org.

[9] Kee, R. J., Rupley, F. M., and Miller, J. A., "The Chemkin Thermodynamic Database," SAND87-8215B, Sandia National Labs., Albuquerque, NM, March 1990.

[10] Gracia-Salcedo, C. M., Brabbs, T. A., and McBride, B. J., "Experimental Verification of the Thermodynamic Properties for a Jet-A Fuel," NASA TM-101475, Sept. 1988.

[11] Freeman, G., and Lefebvre, A. H., "Spontaneous Ignition Characteristics of Gaseous Hydrocarbon–Air Mixtures," *Combustion and Flame*, Vol. 58, No. 2, Nov. 1984, pp. 153–162.

[12] Chang, J. S., and Lewis, M. J., "Development of a Jet-A/Silane/Hydrogen Reaction Mechanism for Modeling a Scramjet Combustor," *AIAA Paper 99-2252*, presented at the 1999 AIAA/ASME/SAE Joint Propulsion Conf., Los Angeles, CA, June 1999.

Lithium Peroxide Fuel Cells for Electric Vehicle Propulsion

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Introduction

A PROPULSION system consisting of a compact electric motor and one or more lithium-based fuel cells (Li–water, Li–hydrogen peroxide, Li–air) holds considerable promise as a nonpolluting, recyclable-fuel power plant for airplanes, uncrewed air vehicles (UAV), helicopters, automotive vehicles, and surface water vehicles. The technology has its roots in U.S. Navy electric torpedo research done in the 1970s by Lockheed (see Refs. 1–3) and subsequent classified Defense Advanced Research Projects Agency-sponsored research in the 1980s for an uncrewed reconnaissance aircraft.

Recent studies[4] have shown that the gasoline-fueled propulsion system of a typical 225-hp light airplane could be replaced with an electric-motor, lithium–air fuel cell power plant developing the same power and the same endurance with approximately the same weight. The by-product of producing electricity in the fuel cell is lithium hydroxide (Li–OH), which would be retained onboard and recycled after flight to retrieve the metallic lithium for reuse. Furthermore,

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lithium compounds, including easily mined salts, are abundant in nature, much more so than petroleum (lithium is the 18th most abundant element in nature). Also, the process for extracting the metallic lithium is well known.

The objective of this paper is to design a Li–hydrogen peroxide fuel cell and evaluate its performance in a small-scale laboratory setup. The goal is to identify the design parameters affecting the performance of the fuel cells and also to evaluate their performance against the theoretical predictions. This project has been initiated as a first step toward designing and fabricating a much more complex Li–air fuel cell system that has the specific energy closer to that of a gasoline–air system but is two to three times more efficient. The performance and cost benefit studies, using Li–H_2O_2 fuel cells for propulsion, are also performed for a general aviation (GA) Beech Bonanza Model 45 airplane and for an airplane for Mars exploration (AME). The successful demonstration of this technology will be a major milestone toward the ultimate goal of developing a cost-effective, emission-free propulsion system for ground, air, and surface water vehicles.

Why Lithium-Based Fuel Cells?

As shown in Table 1, Li-based fuel cells, especially the lithium–air fuel cells, have the potential for superior performance to internal combustion engines and other electrochemical- or hydrocarbon-based systems. Lithium–air has a theoretical specific energy more than 78 times that of a lead–acid battery. Thus, the combined attributes of low oxygen requirement, ultra-high-power density, and zero emissions make lithium–air fuel cells an attractive power source for air vehicles.

Principle of Operation

The basic principle of operation of a single Li–water fuel cell is shown in Fig. 1. The anodic dissolution of Li comprises the following electrochemical reactions.

Anode reaction:

$$2\mathrm{Li} \rightarrow 2\mathrm{Li}^+ + 2e^- + 3.02\ \mathrm{V} \tag{1}$$

Cathode reaction:

$$2e^- + 2\mathrm{H_2O} \rightarrow \mathrm{H_2} + 2\mathrm{OH}^- - 0.83\ \mathrm{V} \tag{2}$$

The sum of these two reactions, the parasitic reaction, is given as

$$2\mathrm{Li} + 2\mathrm{H_2O} \rightarrow 2\mathrm{LiOH} + \mathrm{H_2} + 2.19\ \mathrm{V} \tag{3}$$

Table 1 Energy characteristics of various power sources[2]

System	Specific energy, kW · h/kg	Efficiency, %
Lithium–air	13.3	50[a]
Gasoline–air	12.4	25
Aluminum–air	8.2	45
Lithium–hydrogen peroxide	4.4	67
Lithium–water	2.4	50
Lithium–thionyl chloride	1.5	70
Lithium–silver oxide	1.4	50
Nickel–cadmium	0.24	14
Lead–acid	0.17	18

[a]Efficiency at peak power, Li–air fuel cell efficiency increases to better than 90% as power is decreased below maximum.

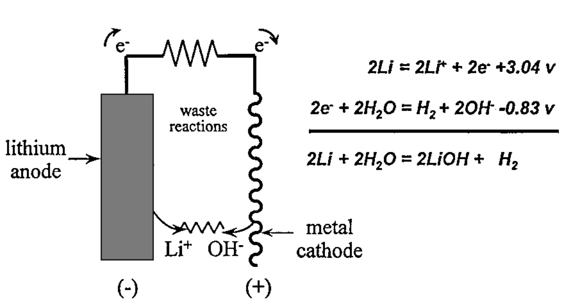

Fig. 1 Basic principle of operation of Li–H_2O battery.

As can be seen from Eq. (3), a single Li–water fuel cell theoretically generates 2.19 V. The electrochemical reactions in a Li–air fuel cell can be described as follows.

Anode reaction:

$$2\mathrm{Li} \rightarrow 2\mathrm{Li}^+ + 2e^- + 3.04\ \mathrm{V} \tag{4}$$

Cathode reaction:

$$2e^- + \mathrm{H_2O} + \tfrac{1}{2}\mathrm{O_2} \rightarrow 2\mathrm{OH}^- + 0.4\ \mathrm{V} \tag{5}$$

The parasitic cell reaction then becomes

$$2\mathrm{Li} + \mathrm{H_2O} + \tfrac{1}{2}\mathrm{O_2} \rightarrow 2\mathrm{LiOH} + 3.44\ \mathrm{V} \tag{6}$$

The electrochemical reactions in a Li–hydrogen peroxide fuel cell can be described as follows.

Anode reaction:

$$2\mathrm{Li} \rightarrow 2\mathrm{Li}^+ + 2e^- + 3.04\ \mathrm{V} \tag{7}$$

Cathode reaction:

$$2e^- + \mathrm{H_2O} + \mathrm{H_2O_2} \rightarrow 2\mathrm{OH}^- + \mathrm{H_2O} + 0.88\ \mathrm{V} \tag{8}$$

The overall cell reaction then becomes

$$2\mathrm{Li} + \mathrm{H_2O} + \mathrm{H_2O_2} \rightarrow 2\mathrm{LiOH} * \mathrm{H_2O} + 3.92\ \mathrm{V} \tag{9}$$

Fuel Cell Design, Experimental Setup, and Results

The design of the fuel cell is the most important part of the process in building an efficient fuel cell. One must achieve a balance between the electrolyte flow rate (the ability for the water, LiOH, or peroxide to pass through both the anode and cathode) and the contact pressure (the pressure between the lithium anode and the platinum cathode must be high enough to create current, but low enough to allow electrolyte flow) to attain maximum efficiency. The materials used to create those effects of contact pressure and electrolyte flow must also be able to withstand the heat created by the reaction of lithium with water, LiOH, or hydrogen peroxide. One also has to take into account the safety requirements and the ability to control various parameters such as electrolyte flow rate, electrolyte concentration, electrolyte temperature, and anode–cathode contact pressure. We designed a six-cell Li–H_2O_2 battery to run a 12-V, 450-W motor. This battery was designed to fit the fuselage of a radio-controlled (R/C) Electric Telemaster 40 aircraft. Using the theoretical output of one fuel cell, it was determined that approximately six fuel cells connected in series with each cell outputting 2.19 V would be needed. Then, by considering the power requirements of the motor, 450 W, the number of watts needed per cell is 75 W. Using both the power and the voltage requirements, the current needed to run the motor is 37.5 A. Then, using the known range of current densities of a lithium-based fuel cell (approximately 500–1500 ma/cm^2), it was concluded that a cell of size 2.75 × 5.5 in would suffice. The six fuel cells would fit in a volume of 3 × 5.75 × 7 $in.^3$, which is available in the fuselage of the R/C aircraft. Using these measurements, a plexiglass box with six slots was designed and manufactured to hold the fuel cells. Stainless steel wire mesh with measurements 2.75 × 5.5 in. was used for both the anode and cathode. Platinum was used as the cathode. For this purpose, stainless steel wire mesh was plated with 20 μin. of platinum.

A special environment that had 0% humidity, 0% nitrogen gas, and 0% oxygen gas was created for handling the lithium. A 0.06 in thick lithium sheet was used as the anode. The platinum mesh and lithium foil were screwed together with plastic screws. A 4 molar solution was used as the electrolyte to start the reaction. The fuel cells were connected in series. A bench test apparatus (including a dynamometer) was designed to obtain measurements of voltage, current, revolutions per minute, temperature, pH, force, torque, and thrust. The details of the fuel cell design and experimental setup are not given here, but can be obtained from Ref. 5.

As a first step, experiments were performed for a single cell because the single cell environment was easily controllable with respect to the four critical parameters that affect the fuel cell performance: electrolyte flow rate, electrolyte concentration, electrolyte temperature, and anode–cathode contact pressure. Multicell environments were difficult to control with respect to these parameters in our simple experimental setup. It can be seen from the data in

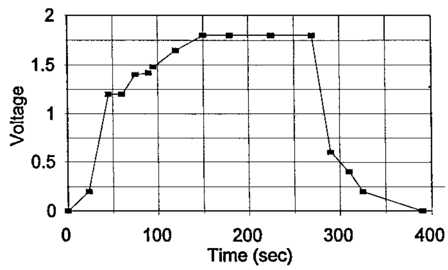

Fig. 2 Voltage vs time (single cell).

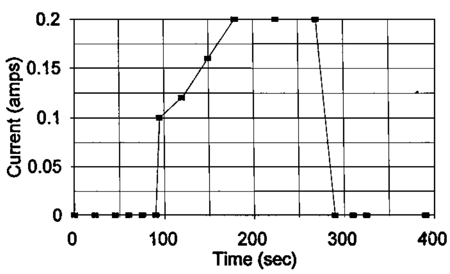

Fig. 3 Current vs time (single cell).

Figs. 2 and 3 that the maximum voltage generated is 1.8 V and the maximum current is a 0.2 A. The theoretical possible voltage is 2.19 V without any losses. Because the single cell was connected to a 10-Ω resistor, the expected current is as obtained. Furthermore, the variation of voltage and current with time is similar to that reported in Ref. 1. These results establish the success of the single cell experiment.

Case Studies

$Li-H_2O_2$ Fuel Cells for a General Aviation Aircraft

Table 2 shows the typical flight profile of a Beech Bonanza Model 35 GA aircraft. Table 3 shows the weight comparison for delivering 337 kW · h. The takeoff weights of a gasoline-powered propulsion system and a $Li-H_2O_2$-powered system are comparable. This study shows that a $Li-H_2O_2$ fuel cell powered propulsion system is comparable in performance to the standard gasoline-powered propulsion system but has a significant advantage in being emission free.

$Li-H_2O_2$ Fuel Cells for an AME

Design of propulsion system for an AME provides significantly different challenges than that for GA and UAV applications. It is due to the rarefied atmosphere of Mars, composed predominantly (95.5%) of carbon dioxide in contrast to the standard Earth atmosphere, composed of air. To design a propulsion system for the Mars flyer using $Li-H_2O_2$ fuel cells, the mission requirements for AME would have to be specified. Table 4 gives the power and energy requirements for a typical mission of two 5-h flights for AME.

The $Li-H_2O_2$ propulsion system for AME will have three parts: a cell stack, an oxidizer reservoir, and a reactor/storage system. Each of these parts would have to be sized for the AME mission. A 30-V propulsion system appears to be adequate for the proposed mission that will require a stack of 13 2.4-V cells.

To generate 63 kW · h of energy to provide 6.3 kW of power to the motor for 10 h, the fuel cell will require 6.6 kg of lithium and 20.1 kg of hydrogen peroxide. For ground operations over a period of 1500 h (60 + Earth days), the AME will require 50 W of continuous power with total energy requirement of 75 kW · h, as shown in Table 4. This added item will require another 7.9 kg of lithium and 23.7 kg of hydrogen peroxide. Table 5 tabulates the lithium, hydrogen peroxide, and total weight requirements.

It appears that a $Li-H_2O_2$ fuel cell based propulsion system can be effective for in-flight operations if the atmospheric carbon dioxide can be used in power generation and the lithium carbonate thus generated can be expelled from AME. For ground operations, it appears more beneficial to carry a solar-electric array and a rechargeable battery.

Table 2 Typical flight profile of a 1947 Beech Bonanza Model 35

Parameter	Takeoff	Climb (8000 ft)	Cruise	Descent landing	Totals
Power, hp · kW	205	154	103	50	——
	153	115	77	37	——
Duration, min	1	10	<240	15	<266
Energy, kW · h	2.55	19.2	<306	9.3	<337
Speed, mph	0–70	100	175	175	——
Range, mile	<1	16	700	45	765

Table 3 Weight comparison for delivering 337 kw ·h

Parameter	Gasoline-powered piston engine, kg	$Li-H_2O_2$-powered elecric motor, kg
Consumables		
Fuel	136	44
Oxidizer	——	218
Prime mover		
Motor	205	45
Motor components	14	7
Auxiliary systems	27	100
Total	382	415

Table 4 Mission requirements for a Mars flyer

Operations	Power, kW	Duration, h	Energy, kW · h
In-flight	6.3	10 (2 × 5)	63
Ground	0.05	1500	75

Table 5 Weight requirements for a typical mission for Mars flyer

Operation	Li, kg	H_2O_2, kg	Total, kg
In-flight (10 h)	6.6	20.1	26.7
On ground (1500 h)	7.9	23.7	31.6
Complete operation	14.4	43.8	58.3

Conclusions

Small-scale lithium–hydrogen peroxide fuel cells with output power in the range of 500 W were designed and built. Experiments were performed to evaluate the performance of a single cell. For a single cell, the experimental performance data were close to theoretically expected results. This work is a first step toward designing and fabricating a much more complex Li–air fuel cell system that has the specific energy closer to that of a gasoline–air system but is 2–3 times more efficient and is emission free. The case studies for a GA aircraft and an AME show the performance, cost, and environmental benefits of Li-based fuel cells for electric propulsion.

Acknowledgments

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References

[1]Galbraith, A. D., "Electric Propulsion for High Performance Aircraft," AIAA Paper 79-1265, 1979.

[2]Galbraith, A. D., "Electric Propulsion for Light Aircraft II: Lithium-Air Fuel Cell for Primary Power," National Institute for Aviation Research, Wichita, Kansas, NIAR Rept. 96-3, Nov. 1996.

[3]Momyer, W. R., "Lithium/Hydrogen Peroxide Battery for Torpedo Propulsion," Lockheed Missile and Space Co., Sunnyvale, CA, Rept. LMSC/D556381, April 1977.

[4]Foch, R. J., "Electric Propulsion for Experimental and General Aviation Aircraft," *Proceedings of the Experimental Aircraft Association's Annual Convention*, Oshkosh, WI, Aug. 1996.

[5]Agarwal, G., "Lithium–Peroxide Fuel Cells for Electric Propulsion for an Airplane for Mars Exploration," AIAA Paper 99-2356, 1999.