SENSITIVITY ANALYSES OF PEM FUEL CELL SYSTEMS
FOR BOTH
OPEN AND CLOSED LOOP APPLICATIONS

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ABSTRACT
A specialized computer modelling technique has been developed to evaluate fuel cell systems as possible candidates for various commercial applications. The computer model includes reactants and products chemistry, storage, electrochemical energy conversion efficiency, and the possibility of using seawater as a reactant. The results clearly indicate superior energy capacity for lithium hydride (LiH), lithium aluminum hydride (LiAlH₄), or calcium hydride (CaH₂) fuels with liquid oxygen (LOX) compared to all of the non-metal hydride fueled systems considered, including those using liquid oxygen with aluminum (Al/LOX) and methanol (CH₃OH/LOX) systems. A description of the computer model is given and sensitivity results of various studies are reported.

In the hydride studies, water is assumed to react directly within a hydride fuel tank to produce the hydrogen gas required for operation of the fuel cell. The hydroxide product formed by this reaction remains in the tank. The tanks have been sized to include the effects of a possible larger volume required for the product (as in the case of CaH₂ and NaBH₄/LOX). Sensitivity studies are included that contrast applications to an open loop system with no chemical product retention, a closed loop system with product retention and the various effects of system efficiencies, assumed filter cake volume fractions, and tank shapes.

INTRODUCTION
A DARPA/Navy Unmanned Underwater Vehicle (UUV) energy technology program has recently begun to consider the use of fuel cells to replace existing silver-zinc batteries for general UUV applications. The goal of this particular program is to achieve a factor of three-to-ten more energy storage within the allotted battery compartment volume of the UUV.

During an investigation of the feasibility of fuel cells to replace batteries for such applications, a detailed computer program was written to model and compare any number of given fuel cell systems for similar applications. The program is written as a large spreadsheet, and includes all of the data required to model the chemistry of each fuel cell system, various assumed system parameters, such as the system's efficiency, and calculates each system's required mass and volume. In order to size each given system for a given particular application, an iterative procedure is used to calculate what the tank sizes and volumes are required in order to achieve a given system energy. Thus, given a system size or volume constraint, the model then determines the maximum possible size of the various subsystems and tanks to fit the given application, and calculates the maximum energy available to placed within that given space.

SYSTEM SIMULATION
A large number of fuel cell systems were considered in the analyses. A detailed description of these systems and the chemical reactions involved with each system is given in a companion paper. [1] A number of other comparative analyses have also been reported which also studied possible various fuel cell and other energy systems for UUV applications. [2-4] These energy systems generally fall into two groups: (1) fuel cells using hydrogen or methanol fuel with oxygen and (2) semi-metallic fuel cells using consumable aluminum or lithium electrodes with oxygen, hydrogen peroxide, or water. A detailed discussion of the chemistry of the reactions of the various fuel cell systems studied is given in reference 1.

A flow diagram of the calculational model is given in Fig. 1. The calculations are performed on a large spreadsheet program on a personal computer, thus making additions and modifications to the calculations very easy. Each fuel and oxidant system is modeled in a separate column of the spreadsheet, and all physical, chemical, and chemical reaction properties are stored in rows for each system. The chemical reactions for each fuel cell system define these given system data. Then, given a desired energy capacity for each system (in each column), the calculations proceed to calculate the required weight of the fuel, oxidant, additional reactants, and all of the products (which may be more than one in some cases). Tank weights and total required volumes are then also calculated in various rows of the spreadsheet. Given the geometrical shape of the fuel and oxidant tanks, and the size and shape of the fuel cell and additional components used, the calculations proceed to determine the total system volume and total system length needed by that fuel cell system to yield the given energy capacity. These are then compared to given system constraints, such as the allowed system volume and length. The appropriate comparisons are automatically made, and the calculations then proceed to iterate by adjusting the assumed energy of each system. Convergence is obtained to the nearest kilowatt-hour.
A library of complex macros is used to perform the convergence calculations. In this manner, each energy system (in each column) can be contrasted and compared to any other given energy system on an equal energy or equal system volume or length basis. Sensitivity analyses can then be made to determine the effects of various system constraints on the applicability of those energy system for that application.

ENERGY SYSTEMS CONSIDERED

A listing of some of the energy systems considered in this study is given in Table 1. Standard chemical element abbreviations are used throughout the remainder of this paper. The fuels and oxidants for each fuel cell system are listed along with the required chemical reaction reactants and products. Also listed are the electrolytes used for each product when filter cakes are included in the model. Cryogenic liquid oxygen (at 71.2 lbs/cu. ft.) is used in some systems and is abbreviated as LOX.

Particular detailed attention has been given to the chemical definitions of each system. For example, when using the lithium borohydride (LiBH4) in a fuel cell system, a non-trivial amount of formic acid is required to be included in the calculations to complete the chemical reactions. Also, the 90% concentration of hydrogen peroxide (H2O2) used in the aluminum-hydrogen peroxide energy system is explicitly included in these calculations.

SYSTEM CONSTRAINTS

The system constraints incorporated into the logic of the computer program are listed in Table 2.

SYSTEM COMPARISONS

Four system comparisons are presented. All results are given in terms of an "Energy X Factor," which is defined as the amount of energy available to be produced by each system normalized to 336 W-Hr. This normalization constant is an optimistic estimated amount of energy currently provided by current silver-zinc batteries in UUV applications.

The first system comparison contrasts the ability of these energy systems to provide available energy to a given UUV with a known volume, length, and weight constraints. Given the UUV, the maximum size and thus the maximum amount of energy able to be produced can be plotted for each system. In Fig. 2, the amount of energy allowed to be placed within a UUV is plotted for five cases: (A) allowing for only fuel, oxidants, and a fuel cell unit, (B) including all the required reactants (representing an open system), (C) including all products (as required in a closed system) and stored separately, (D) including an additional filter cake volume taken to be equal to 25% of the calculated product volume, and including an electrolyte in the filter cake volume voids, and (E) case D where all the products are stored within the fuel or reactant storage tank wherever possible. By comparing the results of the relative five histograms of a given energy system for each of these five cases, it is seen that as the reactants, products, and filter cakes are included in the calculations, the amount of energy available to be placed in the same volume decreases, and for some systems this decrease is rather drastic. It is also noted that a significant energy gain is seen (as expected) when the products are placed into existing storage compartments wherever possible. In some cases, this requires oversizing the size of the reactant or oxidant storage tanks at the beginning of life of the system due to the differences of the initial and final densities. The results indicate that the lithium hydride, lithium aluminum hydride, and calcium hydride systems offer a 6 to 10 X gain over existing silver-zinc batteries for a closed loop application (Case E). It is felt that the borohydrides will require acid and that the sodium systems may prove to be unsafe for UUV use.

The second system comparison contrasts the effect of the system efficiency on the energy storage capability of each system. Using the same constraints as in the first comparison using Case E above, three cases were considered: using system efficiencies of 80%, 100%, and 120% of the efficiencies used above. These results are given in Fig. 3 in Cases A thru C, respectively. As expected, it is seen that the energy capability of each system is directly proportional to its overall efficiency. However, it is interesting to note that this dependency on the efficiency of the system is more dominant in some of the systems than in others.
The third system comparison contrasts the effect of varying the size of the assumed filter cake volume of each system. As in the comparisons of the system efficiencies, the filter cake volume of comparison 1 Case E is varied by 100%, 110%, and 120% to yield the three Cases A thru C as shown in Fig. 4. The energy systems that do not require the use of a filter cake do not show any dependence in this comparison.

The fourth comparison illustrates an effect of storage tank shape. In the design of a cylindrical UUV compartment, more volume may be stored in a toroidal tank shape with an internal cylindrical storage compartment than in a cylindrical tank shape with a cylindrical storage compartment at one end. An analysis was performed to determine the ratio of the volume of the toroidal tank to the volume of the cylindrical tank for a typical sized DARPA UUV application. The volume ratio results are given in Fig. 5 as a function of the length of the storage compartment.

CONCLUSIONS

A computational spreadsheet analysis model has been developed for the equal comparison of various energy systems, and in particular fuel cell systems. The model allows the user to quickly compare competing fuel cell system technologies for applications to both open and closed loop systems, and to analyze the effects of varying virtually any system parameters. The approach is very robust and allows for various sensitivity analyses to be performed in order to determine critical design parameters effecting the design and operation of each system. Optimal system designs can therefore be determined for various applications.

It is found that the inclusion of chemical reactants explicitly in the calculations can significantly reduce the energy capability of some of the systems considered (Case A vs. Case B in Fig. 2). An open system is modeled by Case B in Fig. 2 in these results. In a closed system, the reaction products must be stored and the energy capability of the systems is further reduced (Cases C and D in Fig. 2). Allowing the products to reside in oversized fuel tanks gives the maximum possible energy capability of each system (Case E in Fig. 2). The design of a filter cake for product retention is important in the system design and does affect the energy capability of the system (Cases A thru C in Fig. 4). The effects of system efficiency and storage tank shapes and volumes are also of importance when designing such energy systems for diverse applications.

REFERENCES

Fig. 2. Relative Energy Capacities as a Function of Reactants, Products, and Storage Options Considered (Cases A thru E: refer to the text)

Fig. 3. Relative Energy Capacities as a Function of System Efficiencies Considered (Cases A thru C: 80%, 100%, 120% of the Fig. 2 Case E System Efficiency)
Fig. 4. Relative Energy Capacities as a Function of Filter Cake Volume Fractions Considered
(Cases A thru C: 100%, 110%, and 120% of the Fig. 2 Case E Filter Cake Volume)

Fig. 5. Volume Fraction of a Toroidal Tank to a Cylindrical Tank,
for an Equal Length Compartment, Inner Diameter Cavity,
as a Function of the Space Length at the End of the Cylindrical Tank
(Max. Length = 40 in, Dia. = 39.5 in., Inner Dia = 16 in.)