Fuel Cell System Models for U.S. Navy Shipboard Application

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The U.S. Navy's Office of Naval Research (ONR) has sponsored an Advanced Technology Development program to demonstrate a Ship Service Fuel Cell (SSFC) electrical generator in the marine environment. Under this program, a 625 kW Molten Carbonate fuel cell generator, and a 500 kW Fuel Processor, designed for PEM fuel cell applications, are being demonstrated. Both systems are focused on demonstration of a fuel cell based ship service generator utilizing NATO-F76 logistics fuel to produce power with high system fuel efficiency even at partial loads. In addition, ONR is sponsoring advanced research in power dense fuel reformers and processors, hydrogen separation membrane technology and improved sulfur adsorbents with the objective of increasing system power density.

Benefits of fuel cell generators to ship operations include reduced fuel consumption at full and partial loads, smaller intake and exhaust ducting, and reduced thermal and acoustic signatures. The 500 kW Fuel Processor demonstration has been completed. The 625 kW Molten Carbonate fuel cell demonstration is in progress. ONR and Naval Sea Systems Command (NAVSEA) are sponsoring numerous Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs to develop and demonstrate higher performance materials, processes and hardware. These demonstrations will provide higher performance capability than exists in currently demonstrated hardware, and enable a compact shipboard installation.

The technology development programs are addressing numerous areas of process improvements. In the area of hydrogen separation, palladium-, silica-, and carbon-based hydrogen separation methods are being developed under contracts with Analytic Power Corporation, Media and Process Technology, and Power and Energy Corporation. Advanced Cooling Technologies, Energent Technologies, General Vortex Energy, and Touchstone Technologies are developing air compression, gas and liquid-fuel combustion, and passive thermal management techniques. Reformer improvements and sulfur tolerant catalysts are being developed by Precision Combustion, and NexTech Materials. Naval logistic fuels contain high levels of sulfur, and considerable progress is being made in the areas of sulfur tolerance and sulfur removal under contracts with Altex Technologies, Pennsylvania State University, Mesoscopic Devices, Fuel Cell Energy, Celltech, Ceramatec, and Physical Optics. High performance and sulfur sensitive solid oxide fuel cells (SOFC) are being developed under contracts with Franklin Fuel Cells and Ion America. Additionally, the Navy is looking to examine contaminant resistant high-temperature PEM fuel cells for their impact on system size and complexity.

As the technology development efforts proceed, it is necessary to evaluate the capabilities, and assess the system impacts of the specific technologies. Prototypes of the various components will be delivered to the US Navy for performance verification and durability testing in US Navy laboratories. In addition, we are developing process models in various configurations, to compare the benefits of the technologies. The models critically examine process benefits of various improvements, both separately and in combination, on a system basis. The following sections of this paper describe the approach we have taken, the modeling environment and procedures, and some preliminary findings.

Modeling of fuel cell technologies encompasses a wide variety of components, layouts, and potential integration schemes. Accumulated “lessons learned” from the SSFC program showed the need to improve volumetric power density by 3-4X, reduce system complexity, enable fuel cell stack technology to operate in a Navy environment, the need for higher fuel preprocessing capability to remove sulfur and the ability to enable use of multi fuels, and reforming and hybrid air system technologies to adapt configuration based on specific application. Consideration must be made for efficiency, as well as transient operation, ship interface requirements, water neutrality, waste product removal, and size. Modeling and simulation must be used to find the optimum balance between system efficiency, complexity, and volume to meet shipboard operational and environmental requirements.

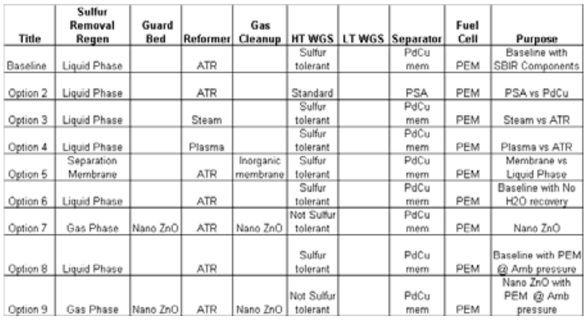
Fuel cell system modeling has been performed using the ASPEN Plus chemical process simulator, and has been evaluated in a pilot and full-scale (500 kWe) size, at steady-state. Systems have been designed and evaluated for use with both NATO F-76 fuel, which has a sulfur content of up to 1% (w), and JP-5, which has a sulfur content of up to 0.3% (w). Fuels consideration is critical for Navy applications, due to the high sulfur content, which has effects on the actual operation of catalyzed systems. Fuels were defined as “pseudocomponents”, based upon their API gravity and average boiling point. Data for typical F-76 and JP-5 fuels was derived from fleet fuel averages measured over many years and thousands of gallons of fuel. Using the pseudocomponent method resulted in the creation of a typical fuel molecule with a specific carbon to hydrogen ratio. For F-76 (average API gravity 34.4) the average typical molecule was C15.01H26.63, and for JP-5 fuel, (average API gravity 41.0), the average typical molecule was C12.40H23.13. However, these surrogate molecules did not include the sulfur species. Based upon data from F-76 and

JP-5 fuels, it was determined that dibenzothiophene (CAS# 132-65-0) was the most typical sulfur carrying species found in Navy logistic fuel. Dibenzothiophene was added to the respective pseudocomponent fuel, in the amount necessary to indicate the desired weight percentage of sulfur.

Individual component modeling was based upon parameters provided by companies producing prototype equipment for the Navy under ONR SBIR and STTR contracts. Overall system operation concepts were derived based upon necessary operating temperatures and pressures, as well as based upon materials, catalyst supports, and separation equipment chosen. Additional consideration was given for air-based reformation schemes for the purpose of minimizing air requirements and for steam-based reformation in order to minimize specific reactions and heat transfer duties which could require sizable or unrealistic equipment.

Primary system models include desulfurization systems, reformers, water-gas shift reactors, separation membranes, and low-temprature or high-temprature PEM fuel cells. Reformers studied included ATR, steam reforming and plasma reformation, of which ATR and plasma varieties are currently being built for Navy testing. Water-gas shift modeling was based upon sulfur-tolerant catalysts currently being designed for the Navy, which operate at higher than normal temperatures. Separation systems studied included palladium alloy, carbon, PSA, and oxygen transport. Separator raffinate, which includes hydrogen, carbon monoxide and methane, was burned for the purpose of providing heat for steam generation. Due to the use of purified hydrogen, low temperature and high temperature PEM fuel cells were assumed to be nearly dead-headed, with utilization rates of ~98%. Operating voltages were determined by OEM data on currently available equipment that will be purchased by the US Navy for testing. Table 1 shows a number of selected models that were produced. Overall, more than 20 models have been created to study modes of integration, component co-operation and efficiency given different equipment layouts.

Table 1: Selected Models



Title	Sulfur Removal Regen	Guard Bed	Reformer	Gas Cleanup	HT WGS	LT WGS	Separator	Fuel Cell	Purpose
Baseline	Liquid Phase		ATR		Sulfur tolerant		PdCu mem	PEM	Baseline with SBIR Components
Option 2	Liquid Phase		ATR		Standard		PSA	PEM	PSA vs PdCu
Option 3	Liquid Phase		Steam		Sulfur tolerant		PdCu mem	PEM	Steam vs ATR
Option 4	Liquid Phase		Plasma		Sulfur tolerant		PdCu mem	PEM	Plasma vs ATR
Option 5	Separation Membrane		ATR	Inorganic membrane	Sulfur tolerant		PdCu mem	PEM	Membrane vs Liquid Phase
Option 6	Liquid Phase		ATR		Sulfur tolerant		PdCu mem	PEM	Baseline with No H2O recovery
Option 7	Gas Phase	Nano ZnO	ATR	Nano ZnO	Not Sulfur tolerant		PdCu mem	PEM	Nano ZnO
Option 8	Liquid Phase		ATR		Sulfur tolerant		PdCu mem	PEM	Baseline with PEM @ Amb pressure
Option 9	Gas Phase	Nano ZnO	ATR	Nano ZnO	Not Sulfur tolerant		PdCu mem	PEM	Nano ZnO with PEM @ Amb pressure

System models were created to be as modular as possible, so that individual components could be used in one system layout or another as necessary. Due to the large number of different layout schemes and equipment, it provided some time-saving results, though often there were slight changes and tweaks necessary in order to optimize operation of the system and not violate materials specifications or thermodynamics. However, the modularization of unit operations did allow for good standardization of equipment layouts and provided clean worksheets that are easy to follow, customize and operate. Figure 1 shows a typical system layout, with autothermal reformer, water-gas shift, a membrane separator, the necessary air management equipment as well as the necessary thermal management equipment.

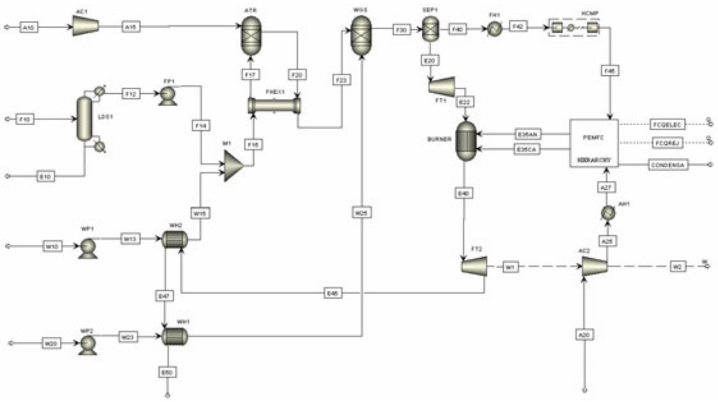


Fig. 1: System Layout including ATR, WGS, Pd-alloy membrane, PEMFC, and all necessary air management equipment.

Typically, systems ultimately achieved a 3:1 steam to carbon ratio. In the case of an autothermal reformer/water-gas shift type system, the reformer was designed to operate at approximately 1:1 steam to carbon, with the remaining water added in the WGS step. For steam reformation systems, a full 3:1 steam to carbon ratio was utilized at the injection and mixing stage, prior to entry into the reformer, to maximize hydrogen production. Careful consideration was made with respect to airflow requirements, due to realistic limitations on oil-less scroll type compression equipment. In order to minimize the airflow requirement in pressurized autothermal reformation systems, oxygen to carbon ratios were kept at 1:1 or less, and preheat of the steam and fuel mixture kept as high as possible through recuperation.

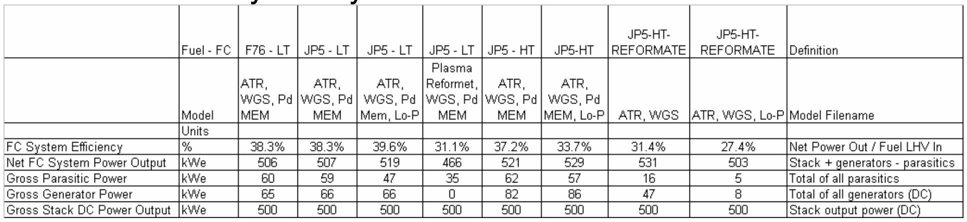
Operating temperatures were maintained per specifications of the products being modeled. The typical preheat of the input components via inline recuperation was approximately 650-675°C for ATR systems, with reactor average temperatures being maintained at 760-780°C. For steam reformer systems, temperature was maintained at approximately 825°C throughout the reactor via the burning of extra fuel. Water gas shift reactor temperatures were adjusted to maintain at approximately 400-425°C; a range necessary for adequate sulfur tolerance. Separation membranes were modeled to be operating at 400°C, and turbine inlet temperatures were controlled so as to not exceed 800°C.

Operating pressures for systems with separation membranes were set to seven atmospheres. This was a necessity due to the requirements of the membrane itself, with a limit on pressure set by available oil-less scroll compression equipment. Fuel cell pressures for both anode and cathode sides were three atmospheres for 'pressurized' fuel cells, and 1.25 atmospheres for 'unpressurized' fuel cells. As the membrane raffnate streams were available at seven atmospheres, it was burned and let down to near atmospheric pressure directly, or, in systems with tighter integration, let down partially, to approximately three atmospheres, then burned and let down further. Anode offgas was not a consideration for any models except high-temperature PEM systems running on reformate, as the systems running on pure hydrogen were assumed to be 'dead headed', with utilization rates in excess of 98%.

Preliminary modeling results indicate that for Navy systems, autothermal reformation with water-gas shift and palladium alloy membranes are a good choice for the combination of sulfur-tolerance, PEM fuel cell longevity, transient operability, system efficiency and power density. The optimal systems utilized ATR reformers with high levels of preheat from recouperation of reformate heat and steam superheating. Preheat was necessary to minimize air requirements, due to the mass and pressure requirements of the system operation, dictated by the palladium alloy separation system. Energy recovery was used whenever possible to enable the production of the necessary steam flowrates and to recover the parasitic losses due to compression. Based upon OEM fuel cell data, low temperature fuel cells provided the best overall system efficiencies, due to their higher operating voltages, and operating the low-temperature PEM fuel cells near ambient pressure provided the highest degree of minimization of parasitics, which is critical to overall system efficiency. The efficiency of such systems is approximately 38-40% (LHV basis), based upon the system models.

Results from other system models indicate that in general, ATR-based systems provide the highest system efficiencies, mainly due to their balanced thermal requirements. Steam reformation based systems performed well also, however their performance was not up to that of the ATR because of the necessity to operate at high temperatures for sulfur tolerance, and the necessity to burn a good deal of fuel in order to make up for the endothermic reaction. Plasma / CPOX reformation provided vastly simplified systems, however, the large amount of waste heat and low hydrogen yields provided poor overall results, due to the need to operate a pure hydrogen stream fed to a PEM fuel cell. Other systems were varied based upon the separation system, and produced poorer results due to the presence of impurities in the gas going to the fuel cell, the loss of pressure in the bulk raffinate stream, steam requirements, etc. Table 2 provides selected results for 500 kWe ATR based hybrid systems, as well as one plasma reformer based system, with both low and high temperature fuel cells, and their respective overall efficiencies.

Table 2: Hybrid System Results and Efficiencies



	Fuel - FC	F76 - LT	JP5 - LT	JP5 - LT	JP5 - LT	JP5 - HT	JP5-HT	JP5-HT-REFORMATE	JP5-HT-REFORMATE	Definition
	Model	ATR, WGS, Pd MEM	ATR, WGS, Pd MEM	ATR, WGS, Pd Mem, Lo-P	Plasma Reformet, WGS, Pd MEM	ATR, WGS, Pd MEM	ATR, WGS, Pd MEM, Lo-P	ATR, WGS	ATR, WGS, Lo-P	Model Filename
	Units									
FC System Efficiency	%	38.3%	38.3%	39.6%	31.1%	37.2%	33.7%	31.4%	27.4%	Net Power Out / Fuel LHV In
Net FC System Power Output	kWe	506	507	519	466	521	529	531	503	Stack + generators - parasitics
Gross Parasitic Power	kWe	60	59	47	35	62	57	16	5	Total of all parasitics
Gross Generator Power	kWe	65	66	66	0	82	86	47	8	Total of all generators (DC)
Gross Stack DC Power Output	kWe	500	500	500	500	500	500	500	500	Stack output power (DC)

Considerations must be made to the models produced, and must be validated in-lab as equipment is delivered to the Navy. Of critical importance is the determination of actual fuel cell operating voltage, and its resultant efficiency. Due to the voltage dependence upon cell area, system size must be considered as a factor in providing high voltages (typically 0.75V) which result in high overall system efficiency. Because system size is a factor, the cell area necessary to provide such voltage may be too large to provide the necessary power density for shipboard use. Similarly, the operational voltage of high-temperature PEM fuel cells must be considered. High-temperature PEM fuel cells offer improved tolerance to impurities, and also offer long-life and high quality waste heat. However, operational voltage is lower than that of typical low-temperature PEM fuel cells, and as a result, system efficiency at steady state is reduced. The resultant longevity, the ability to enhance steam production due to the exhaust temperature, and the reduced thermal and auxiliary requirements may make it an attractive option, particularly if operating voltages can be improved upon.

Currently, ATR reformation appears to be an attractive option for many reasons. However, airflow requirements at full scale may become an issue, in that compression equipment that provides efficient, quiet operation with minimal size, power usage and appropriate turndown does not exist. At the same time, steam reforming is also attractive, because there is no reformer airflow requirement, and hydrogen yields tend to be higher. If sulfur-tolerant steam reformation catalyst, which could operate at lower temperatures was developed, steam reforming could be a very attractive option, and could produce very high efficiencies with less auxiliary equipment. Similarly, catalyst-free systems such as plasma reformation could be very beneficial, due to inherent sulfur tolerance and simplicity. However, ability to operate at pressure and in a wet “ATR mode” must be demonstrated, before they can provide a suitable option for Navy use.

In conclusion, modeling and simulation has proven to be an extremely valuable tool for preliminarily determining what system equipment to pursue for testing and validation. It also provides cost savings and enhanced results, in accordance with DoD guidelines The results obtained thus far based upon preliminary data from several research efforts has enabled insight into system operation, design and integration considerations and also aides in the experimental design for Navy laboratory validation of delivered equipment, which is currently underway. Equipment validation will help to enhance the system models further, and will make the results more realistic, and enable the next necessary step, which is to produce dynamic/transient models and fully characterize power output for integration into electric ship systems.