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ADVANCED SYSTEM ANALYSIS FOR INDIRECT METHANOL FUEL CELL POWER PLANTS FOR TRANSPORTATION APPLICATIONS

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INTRODUCTION

The indirect methanol cell fuel concept actively pursued by the United States Department of Energy and General Motors Corporation proposes the development of an "electrochemical engine" (e.c.e.), an electrical generator capable for usually efficient and clean power production from methanol fuel for the transportation sector. This on-board generator works in consort with batteries to provide electrical power to drive propulsion motors for a range of electric vehicles. Success in this technology could do much to improve impacted environmental areas and to convert part of the transportation fleet to natural gas- and coal-derived methanol as the fuel source. These developments parallel work in Europe and Japan where various fuel cell powered vehicles, often fueled with tanked or hydride hydrogen, are under active development.

Transportation applications present design challenges that are distinctly different from utility requirements, the thrust of most of previous fuel cell programs. In both cases, high conversion efficiency (fuel to electricity) is essential. However, transportation requirements dictate as well designs for high power densities, rapid transients including short times for system start up, and consumer safety. Moreover most studies conclude that costs are more stringent for transportation applications.

The e.c.e. *system* is shown in Figure 1. This hardware is formed from four interacting components: 1.) the *fuel processor* that includes vaporization sections to form gaseous water and methanol and post processing devices to clean the output stream, 2.) the *fuel cell stack* that reacts the product hydrogen with air to generate electrical power, 3.) the *air compression and decompression device* to deliver the cathode air supply at appropriate flow rates and pressures and then recovers some fraction of the pressure-volume work, and 4.) the *condensing cross flow heat exchange device* that results in significant quantities of water recovery so that the water product can serve essentially all of the water input requirements to component 1. (In this way, no water is required as a separate input stream.) This paper will describe status of each of these components, and describe a model that predicts steady state performance of the e.c.e.

1. FUEL PROCESSING COMPONENTS

The fuel processing components operate to generate hydrogen from liquid methanol. This process involves reaction of gaseous methanol and steam on surfaces of heterogeneous catalysts. The energetics for input energy to drive this reaction are demanding. The total fuel energy is based on heat of oxidation of methanol ($\Delta H = -715.4$ kJ/mol). On a mole basis, about 25% of the total energy is required for hydrogen production following the steam reforming route:

$$CH_3OH + H_2O = CO_2 + 3\,H_2$$

The reaction is usually done with excess steam, using a steam to methanol ratio between 1.1 and 1.3. Although earlier studies suggest that steam generation is the primary heat input for this process, analyses show that each of the three required processes, 1.) heating methanol to reaction temperatures, 2.) heating steam to reaction temperatures, and 3.) providing the heat of reaction, require significant and approximately inputs of thermal energy.

The sum for heat of combustion of the three moles of hydrogen produced by this process is slightly higher than the heat of combustion of the one mole of methanol required as the fuel input— steam reforming increases the fuel enthalpy. This means on a joule basis that the methanol to hydrogen conversion is approximately 75% efficient, assuming a processing step with a steam to methanol ratio of 1.3/1.0. (Lowering the steam to methanol ratio improves this situation.) The required thermal input, equal to 25% of the total fuel energy content, can come largely from heat generated in other parts of the e.c.e system. In fact, most of the design challenges in the e.c.e.engineering development involve thermal management to increase system efficiency by moving "waste heat" generated in other parts of the system into the fuel processing components.

In general the overall e.c.e. system efficiency is the product of the fuel cell stack efficiency and the net reformer efficiency, modified by various thermal inputs from nominal values. A stack operating at 0.800 volt/cell has a maximum efficiency of 65%, assuming complete hydrogen utilization in the anode compartment. If this stack is coupled with a fuel processing section that operates with a maximum efficiency of 75%, the overall maximum system efficiency falls to below 50%. The e.c.e. system efficiency can be improved by transferring heat from the fuel cell stack and other ancillary system components into the fuel processing section, thereby decreasing the thermal inputs that come from direct fuel oxidation. In general, the most efficient e.c.e.system is the one that uses the smallest fraction of fuel for direct heat production to drive the fuel processing reactions.

Figure 2 shows a schematic diagram of current fuel processing concepts. The hydrogen generation is accomplished in three steps, 1.) *steam reforming convertor* using forced convection to provide thermal input, 2.) *shift convertor* with the introduction of additional water to cool and lower the CO content, and 3.) *preferential oxidation convertor* to lower the carbon monoxide content to acceptable levels. The first two steps produce reactants in thermodynamic equilibrium, while the third depends upon kinetics for a sharp decrease in carbon monoxide concentrations, a severe poison in PEM fuel cell stacks.

2. FUEL CELL STACK COMPONENTS

Thermal management and water management are two key system aspects of fuel cell stack engineering. Because these PEM fuel cells operate below the boiling point of water, two phase water management is essential. These heat and water management issues are strongly influenced by the temperature, pressure and the flow stoichiometry of the anode and cathode compartments, in addition to the current density, the fuel cell voltage, and the internal stack resistance. To date most PEM fuel cell stacks rely on internal water flow for thermal management. Heat, removed at the stack temperature is produced as sensible heat in a water flow system. Although it is not required, most contemporary stack designs integrate this water flow with internal humidification systems, especially for anode feed humidification. Because of the required high humidification levels in the anode feed (R.H. > 80%), stack cooling occurs during this humidification step.

Water management is complicated by the electroosmotic processes that couple water transport with the anode-to-cathode flow of the proton flux in PEM fuel cells. Although this flow is less than that found during electrolysis processing (the H_2O/H^+ ratio is between 1 and 2), at higher current densities this water transport process causes anode dehydration. Anode moisture levels are replenished in part by a water transport process within the membrane, flowing from cathode to anode. This process is driven by the water gradient between the cathode and anode. Water removal from the cathode is simplified in air breathing systems by the high nitrogen flow rate. Even with relatively low flow stoichiometries (< 2.0), the mass transport rates through the cathode compartment are necessarily high. For instance, a flow stoichiometry of 1.5 results in a flow rate of approximately seven and one half times that necessary only to sustain the cathode processes.

Waste heat from the stack or cathode exhaust is sufficient to vaporize most of the methanol flow. The anode vent stream, assuming a hydrogen utilization rate of 85%, is then available for contributing to the thermal input for water vaporization. Additional waste heat must be discharged, probably through a water-air heat exchanger (not shown).

3. AIR MANAGEMENT COMPONENTS

Pressured air most likely is required in the cathode so that stack operating temperature can be increased. At higher stack temperature the membrane conductivity increases, a condition required for high power density At higher total pressure the steam pressure can also be increased to sufficient levels. Most likely a pressure near 2 bar is the required operating condition. This region permits high stack performance, but does not dictate complex pressure-volume machinery. A simple turbine component similar to an automotive turbocharger can generate the required gas flows and pressures.

The pressure-volume work in the cathode gas exhaust provides in part the required input energy for pressured operation. In the schematic shown in Figure 1, the enthalpy of the air exhaust is increased by introducing the hot gas from the fuel processing burner vent. This "pressured burner" scheme boasts the enthalpic flow through the expander, and in some simulation examples provides full work for the air compression step. If that is not the case then a motor must be used to supplement the power for moving the air compressor.

4. WATER RECOVERY COMPONENTS

Water recovery is required for an efficient system. The alternative is to fuel the system with a "premix" fuel, or to add water during the fueling process along with methanol. The system described here combines the fuel cell cathode exhaust with the combustor exhaust. This concept merges the product water coming from both the electrochemical oxidation processes (fuel cell stack) and the chemical oxidation processes (heat inputs for fuel processing) into one stream. This stream is cooled by cross-flow using incoming air, or through incorporation of methanol vaporization processing in that section (not shown). The overall input water requirements are one third of the total product volume. Water recovered in excess of the input requirements will be discharged once the relatively small storage volume is full.

5. E.C.E. SYSTEM MODEL

The analytical model describes energy and mass flows in this indirect methanol fuel cell. Currently steady state simulations are available. These show these results:

a. *Thermal Management:* A variety of simulations show balanced thermal situations in which the waste heat is sufficient to provide essentially all of the required input energies. Other system heat sources including cooling of power electronics, cooling of drive motors, *etc.* will improve this situation. The fact that the waste streams can be cooled to the boiling point of methanol is an advantage.

b. *System Efficiency:* The system efficiency is a function of fuel cell voltage, assuming a constant hydrogen utilization (85%). Increases in stack voltage efficiency will result in improved system efficiencies at least until high fuel cell voltages are established (> 1.0 V). Depending upon operating conditions, First Law system efficiencies exceed 55%. Under certain conditions, the power output from the expander exceeds compression work.

c. *Transients:* Start up transients are controlled by the thermal mass of the system. With current designs that mass is large, so start up is a slow process. Water vaporization rates are difficult to change rapidly. It is expected that varying the steam generation rate is the current rate limiting step in meeting transients. The compressor-expander system may well not operate well over a wide range of flow ranges, as is required for a load following system. This suggests that some level of battery power, operating as a fuel cell-hybrid system, may be required to permit the e.c.e. system to move swiftly between load points.

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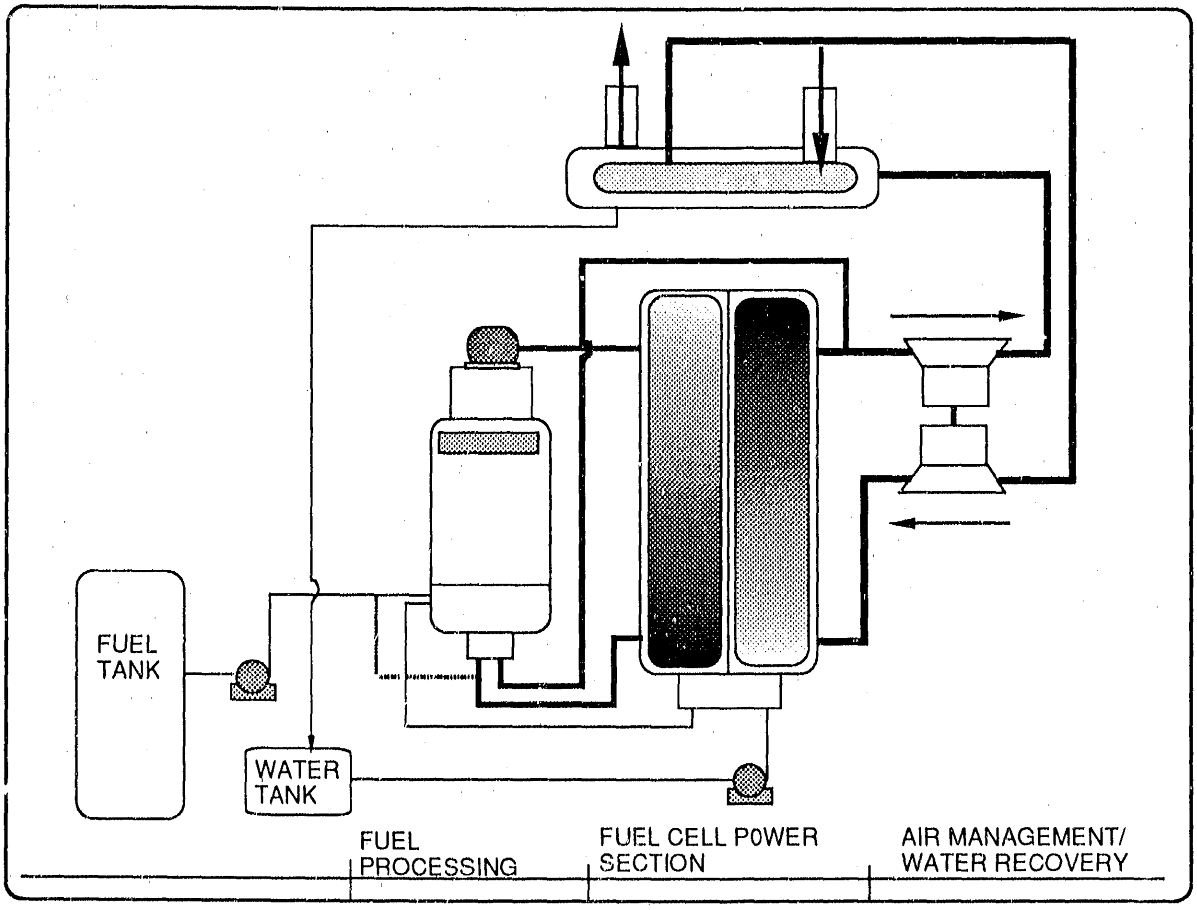

Fig. 1: Electrochemical Engine: This system combines a fuel processing component that generates hydrogen from liquid methanol with a fuel cell power component to generate electrical power. Air management is achieved using a compressor-expander to deliver pressured air. Water recovery involves a cross-flow heat exchanger to preheat the incoming air with the combined exhaust of the system.

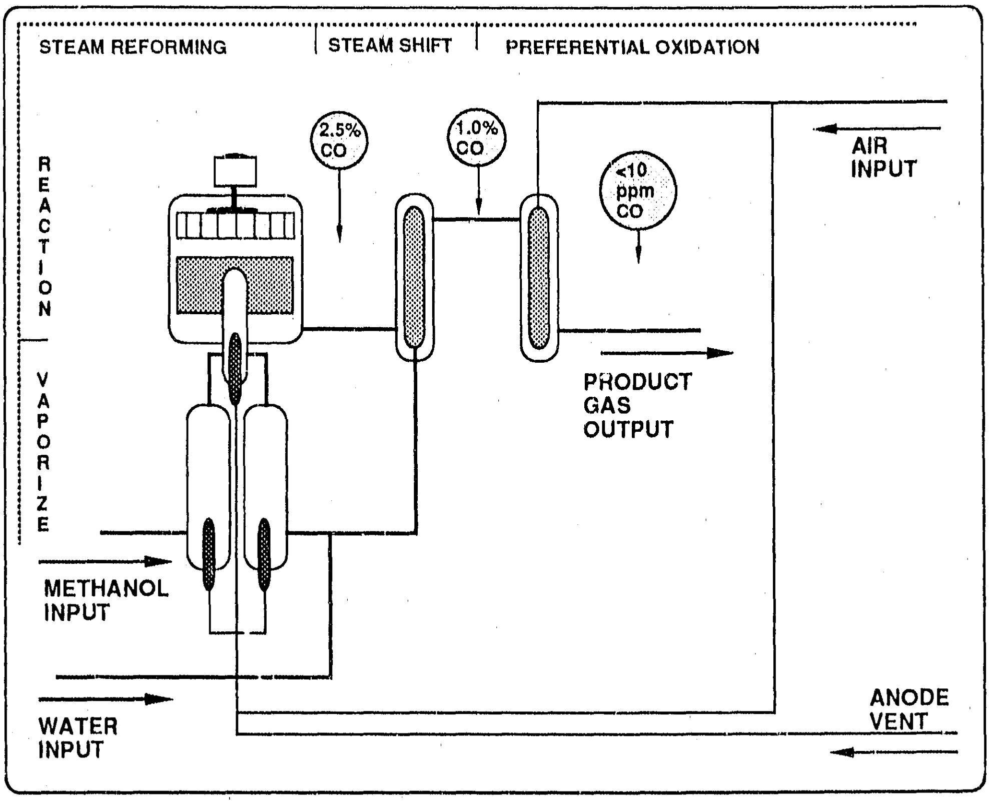

Fig. 2: Methanol Fuel Processing: Fuel processing requires a three sequential process designed to operate on waste streams from the fuel cell stack. Heat is extracted by combustion of the anode vent to drive the water vaporization and system preheat. Vaporized reactants are fed to the steam reforming section. Subsequent processes then 1.) react "breakthrough" methanol and 2.) lower the CO content. The preferential oxidation step also removes other higher molecular weight compounds prior to fuel cell stack feed.

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