Evaluation of a Concept for Hybridizing a Reciprocating Engine with a Fuel Cell

Quarterly Report

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Background

Hybridizing a reciprocating engine with a fuel cell offers some interesting combinations, especially the case where the engine is bottomed by a fuel cell. Ideally, this requires an unusual implementation of the engine – namely, in a rich-burn mode, where syngas (CO, and H2) is produced along with a reduced level of engine power, but with essentially no NOX or particulate. Synergisms are possible because fuel cells generally require some pre-reforming to syngas on the one hand, while on the other, fuel cells may help mitigate emissions that are problematic with engines. Hence, high efficiency and low emissions may be achievable with a more compact and less advanced engine than would be required if the engine where to achieve similar performance on a stand-alone basis. It is hoped this hybrid may be especially useful for distributed power applications as envisioned in EERE's Buildings Cooling, Heating, and Power (BCHP) Initiative.

Process Integration

Aspen simulations were developed to help identify preferred system configurations for the case of a generic high temperature fuel cell (SOFC) integrated with a generic spark ignited, premixed engine operated at various levels both rich and lean of stoichiometric. The options in question refer to the mitigation of engine derived NOX on the fuel side and a tradeoff between catalytic combustion versus high temperature heat exchange on the air side. A schematic showing most of the options is shown in Figure 1. Preliminary results are shown in Table 1, which are based on unfinalized input parameters.

Fuel side options are concerned with the best place to conduct catalytic NOX reduction: (1) in a separate reactor between the engine and fuel cell; (2) in the anode itself; (3) in a separate reactor downstream of the fuel cell. Options 1 and 2 use reformed fuel as the reducing reagent, while Option 3 uses spent fuel. Evaluation of the options is pending the gathering of kinetic data for various temperatures and reducing reagent compositions, as discussed later.

Air side options are concerned with the best way to oxidize spent fuel: (1) combustion in vitiated air downstream of the cathode, most likely in a noncatalytic combustor due to the high temperatures of the fuel cell exhaust; (2) combustion in fresh air upstream of the cathode, possibly requiring a catalytic oxidizer because of the lower temperatures at the fuel cell inlet. Option 2 has the advantage of a significantly smaller high temperature heat exchanger, but with the possible requirements of a catalytic oxidizer and a pressure differential between the anode and cathode to sustain the pressure drop in the oxidizer. Evaluation of these options will primarily focus on the costs of high temperature heat exchange surface versus catalytic oxidizer volume, and on expectations for allowable pressure differentials between anode and cathode.

Engine Performance Modeling

We need to determine the prospects for operating reciprocating engines in the rich region consistent with limits on engine operability. This will include a determination of engine efficiency and cooling requirements for various levels of equivalence ratio while meeting requirements related to autoignition, sooting, and maximum temperature. Our focus will be on homogeneously charged 2-cycle and 4-cycle engines operating on hydrocarbons like natural gas and gasoline.

A trial version of Ricardo's WAVE simulator was used for preliminary validation of the engine modeling approach used in the ASPEN flowsheet simulations, and to identify what added information or modeling capabilities may be needed for feasibility studies of engine concepts. We were able to confirm our representation of a generic Otto cycle in the ASPEN simulations, which yielded results comparable to WAVE predictions for brake efficiency, exhaust temperature, and heat rejection to the cooling system for a cycle operated rich of stoichiometric with standard defaults for friction, heat transfer, valve timing and profiles, and combustion kinetics. The WAVE simulator yielded the expected curves for brake efficiency, NOX, exhaust temperature, and knock intensity, as the equivalence ratio was varied from rich to lean conditions for a variety of fuels such as Indolene (a low sulfur, high octane reference gasoline standard manufactured by Amoco and used for compliance testing) and natural gas. Typical results with Indolene in a generic 4-cycle engine are shown in Figures 2 – 5.

An important issue that was not directly addressable with the basic WAVE simulator was carbon formation. WAVE has built-in predictive capability for carbon formation with direct injection diesel engines, but not for homogenously charged engines. The issue of carbon formation, even at stoichiometric and slightly lean conditions, is an area that will require supplemental modeling capabilities for basic design codes like WAVE. Although carbon is not thermodynamically indicated for the conditions of interest (air-fuel ratio less than stoichiometric, but well above the flammability limit), incomplete combustion, aggravated by wall quenching, lubricant blow-by, and other mechanisms could be at work. To resolve chemical kinetics factors, available codes and data will be evaluated.

It will also be necessary to establish what levels of carbon are tolerable at various locations; mitigation of the fouling of engine cylinders, valves, catalyst beds, and fuel cell internals will need to be considered. Favorable thermodynamics for re-gasifying carbon may be a factor for the components downstream of the engine where low space velocities and other kinetic factors may be at work, but within the engine, short time scales and close tolerances may negate the thermodynamics. Available data on engine operability in the rich region will be sought, as it does not seem likely that predictions can be easily made with available engine simulators.

Transport and Fate of Engine Emissions in Fuel Cell Systems

Aside from power, the desired outputs of the engine are synthesis gas components and sensible thermal energy in the exhaust. Other components in the exhaust include diluents (N2), oxidants (O2, H2O, CO2), and pollutant emissions of nitrogen, sulfur, unburned hydrocarbons, and carbon, in forms and amounts that depend upon the operating mode of the engine. For a basic feasibility analysis, we are primarily interested in the impact and fate of the diluent N2 and the emissions of carbon and NOX.

The impact of N2 diluent on the size of conduits, reactor vessels, heat exchangers, and fuel cells will be accounted for in the process integration studies described above. A key factor that will need to be determined is the space velocity requirement for catalytic NOX reduction under various conditions of temperature and reducing reagent compositions, the same information needed for the comparison of fuel-side system configuration options. A search is underway for available information, and some preliminary data is shown in Table 2. An added determination to be made regarding N2 diluent is a possible increase in the porous electrode gaseous diffusion resistances in the fuel cell.

The issues pertaining to carbon include how much is formed and its properties (size, agglomeration tendency), what the impacts might be on downstream equipment, and what mitigation options exist, if any, taking into account the favorable thermodynamic conditions for re-gasifying carbon. As described previously in connection with engine operability, an estimate needs to be made for the levels of carbon emission at sustainable engine operating modes. This will enable an assessment of the impact on downstream equipment and possible strategies for mitigation, such as barrier filters or reactors and fuel cells with a designed capacity to tolerate certain levels of carbon ("Turning Carbon Directly into Electricity," Lawrence Livermore National Laboratory, S&TR, June 2001).

Related Developments

An invention disclosure was filed at NETL covering certain aspects of the proposed fuel cell-reciprocating engine hybrid, and approval was obtained to proceed. A U.S. patent application is currently being drafted by an assigned attorney. A paper on modeling of fuel cells for advanced energy systems analysis was presented at the Spring 2002 AIChE National Meeting as part of the topical conference on Fuel Cell Technology. Included in the paper was a brief description of advanced hybrid concepts along with an equilibrium calculation to illustrate one of the fundamental motivations for direct partial oxidation reforming in an engine, as shown in Figure 6. How this motivation and others can be reduced to practice is an objective of the upcoming work.

Plans

- Acquire data and technical support in the areas of NOX reduction chemistry, carbon formation in premixed spark ignited engines, and NOX and carbon transport in high temperature fuel cell systems.

- Continue process integration studies and link a customized spreadsheet assessment for performing feasibility studies.

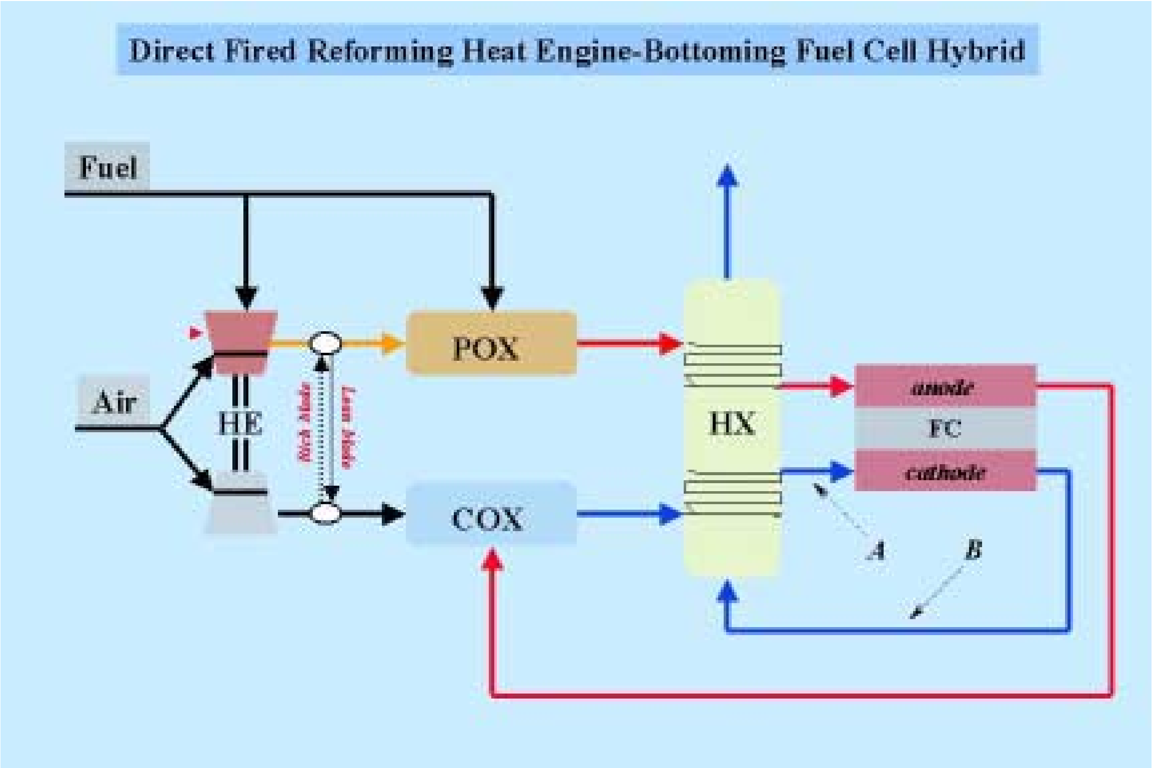

Figure 1. Schematic of major components where actual locations of spent fuel combustion and NOX reduction are optional. Spent fuel combustion is shown occurring in reactor COX upstream of high temperature heat exchanger HX, but COX may be located downstream of HX, before or after the cathode (locations A and B, respectively). NOX reduction options include the POX and COX reactors and the anode itself.

Table 2.
Preliminary Simulation Results;
engine air:fuel equivalence ratio (afr) of 0.75

YIELD	0.43	0.45	*system net power efficiency*
FCFRAC	0.59	0.61	*fuel cell net power fraction*
ICEFF	0.35	0.35	*engine efficiency*
ICERAT	0.75	0.75	*engine afr*
TICE	1800	2000	*engine exhaust temp (F)*
QDUTY	0.04	0.01	*engine heat loss*
TPOX	1405	1375	*pox reformer temp (F)*
POXUSE	0.05	0.01	*pox reformer fuel utilization*
FCUSE	0.85	0.85	*fuel cell fuel utilization*
FCERAT	3.24	5.90	*fuel cell afr*
ECELL	0.70	0.70	*cell voltage (v)*
CDENS	98	188	*current density (mamp/cm^2)*
FCTL	1500	1500	*fuel cell min temp (F)*
FCTH	1849	1768	*fuel cell max temp (F)*
FSPLIT	0.67	0.67	*fuel split fraction to engine*
ASPLIT	0.04	0.01	*air split fraction to pox reformer*
RECYCL	0.01	0.01	*spent fuel recycle ratio*
F-INDEX	0.43	0.45	*system efficiency index*
P-INDEX	1.57	1.66	*system power density index*

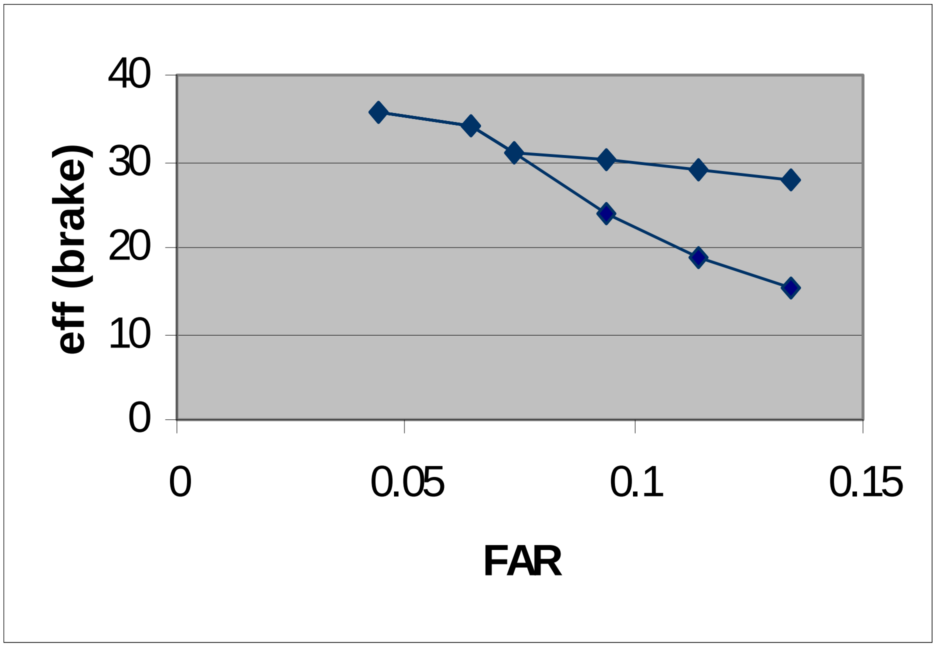

Figure 2. Brake efficiency – upper curve normalized for fuel-air equivalence ratio. WAVE results for generic 4-cycle engine with defaults at 2000 rpm and CR=10.

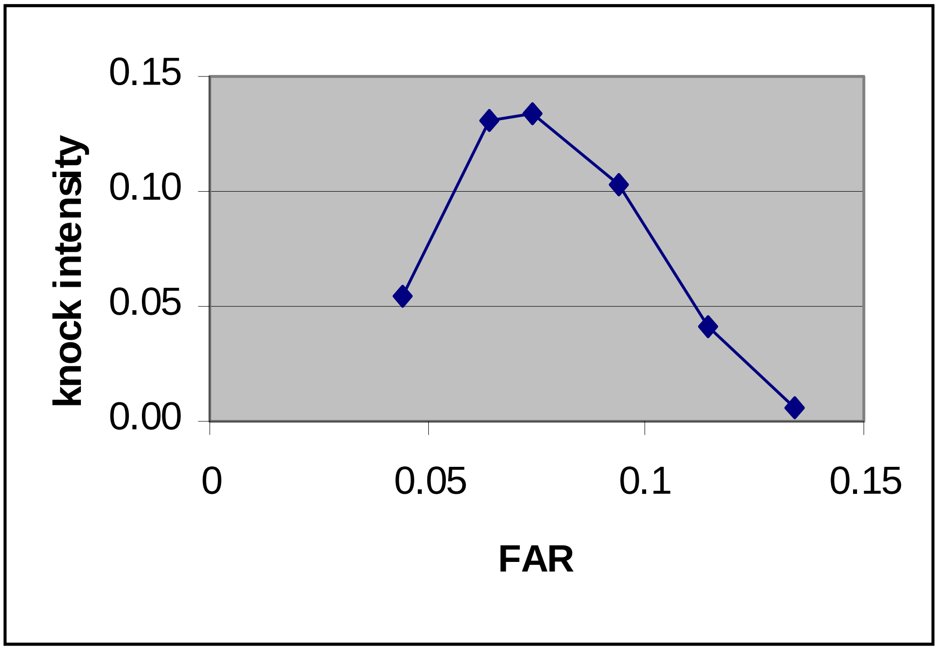

Figure 3. Knock intensity parameter (fraction of fuel unburned at incipient knock). WAVE results for generic 4-cycle engine with defaults at 2000 rpm and CR=10.

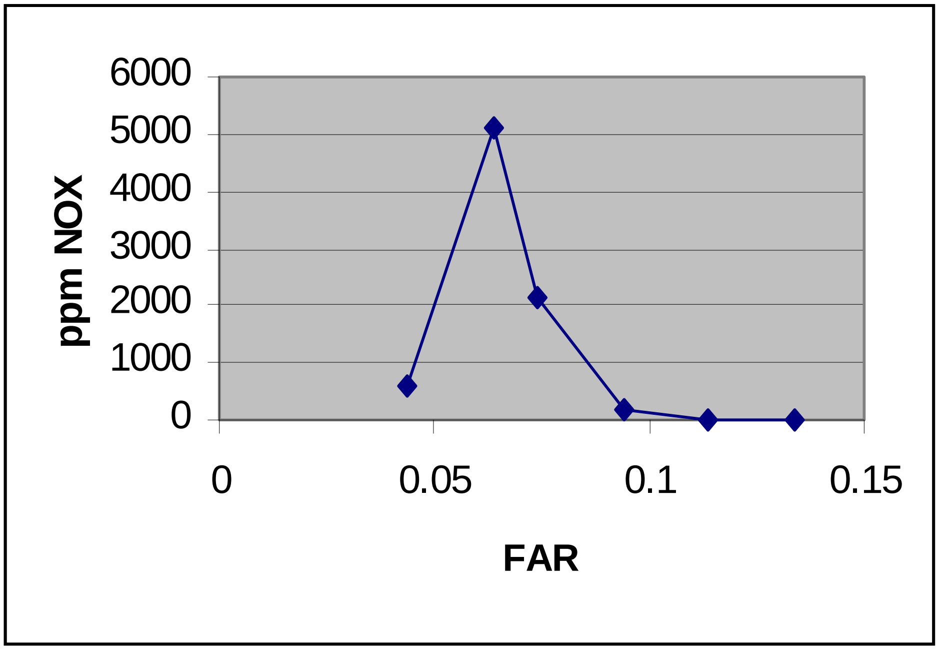

Figure 4. Cycle-averaged NOX emission at engine ports. WAVE results for generic 4-cycle engine with defaults at 2000 rpm and CR=10.

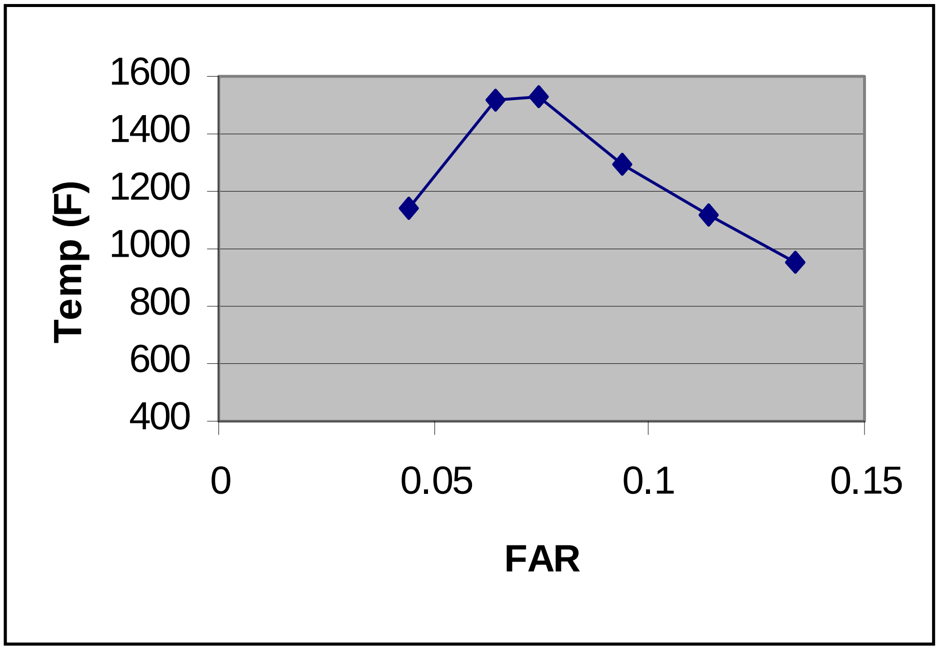

Figure 5. Cycle-averaged engine exhaust temperature. WAVE results for generic 4-cycle engine with defaults at 2000 rpm and CR=10.

Table 2.
Space Velocity Requirements for Common Catalytic Systems
(vol/hr)/vol

Calculated estimate for in-stack reaction at 250 mAmp/cm^2	*SCR (NOX Reduction) ref: KOCAT, Inc. 2001*	*LTS and SMR ref: SRI, H2 Report 1973*	*Calculated estimate for automotive cat. converter*
994	**3,000-20,000**	**1,000-3,600**	**27,936**

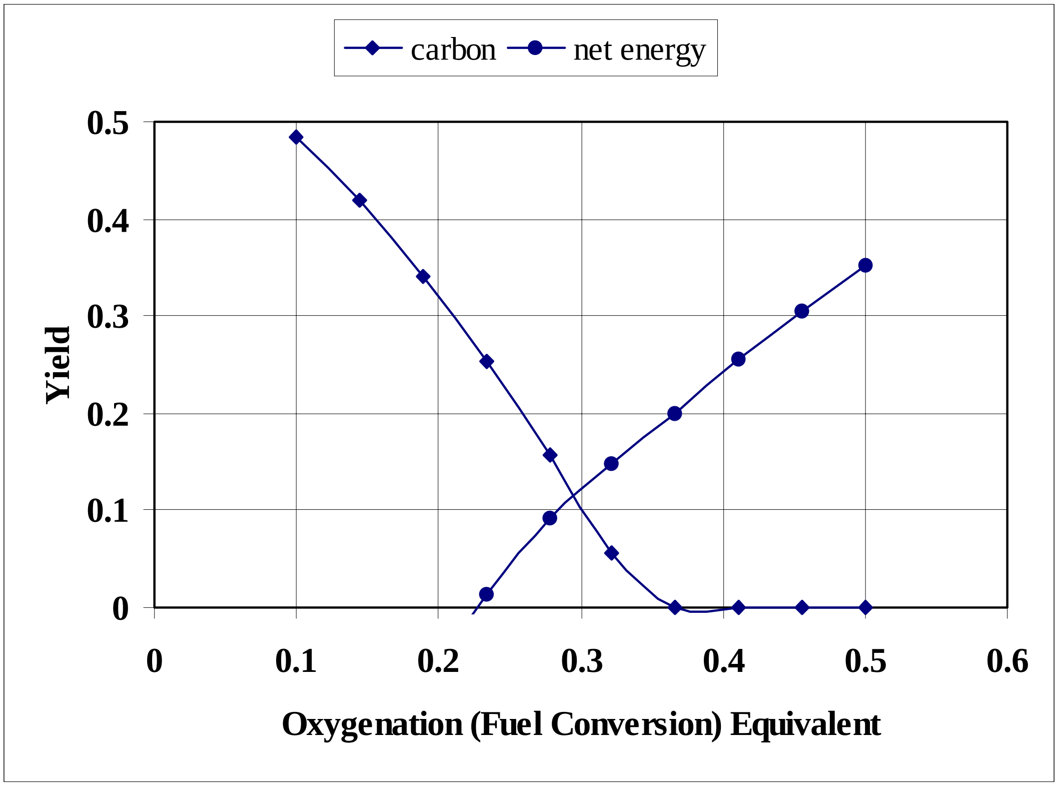

Figure 6. Carbon Yield and Excess Energy Release at Equilibrium for Direct POX Reforming of CH_4 with Dry Air at 1400 F and 10 ATM.