

Use of mixed combustion/electrochemical energy conversion to achieve efficiencies in excess of 70% for transportation-scale engines

Investigators

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Abstract

In order to achieve efficiencies in excess of 70% in transportation-scale engines, a mixed combustion/electrochemical strategy was developed in which a piston engine is coupled to a downstream fuel cell by way of a catalytic reformer. The piston engine serves to reform the fuel and extract some work by operating in a fuel-rich regime, the catalytic reformer serves to catalytically reform the exhaust gas, with additional fuel and water, into a hydrogen-rich syngas, and the fuel cell serves to extract the majority of the remaining chemical exergy in the form of electrical work. Heat exchangers and turbomachinery are also employed to manage the thermomechanical exergy effectively within the system. Modeling results suggest that this strategy can reach the goal of 70% efficiency on an LHV basis. The modeled system that achieves this employs a high-temperature strategy in which a thermally-insulated, compression-ignition engine is coupled to a downstream solid oxide fuel cell through a high temperature reformer. This strategy relies on the capability of the constituent devices (i.e. the engine, the reformer, and the fuel cell) to perform their modeled function, however. Regarding the engine, it must be verified that fuel-rich operation without forming significant non-equilibrium products (soot and hydrocarbons) is possible in a direct-injection, compression-ignition (DI-CI) combustion strategy. Regarding the reformer, it must be verified that commercial catalysts are active and stable in the environment modeled in the system and produce the required product stream for the downstream fuel cell. These two areas are the focus of the most recent research efforts. The investigation of the rich DI-CI combustion strategy consists of the operation of single-cylinder research engine to measure the rich combustion products as well as the work output, optical access experiments in both a single-cylinder optical-access engine as well as an extreme compression device to observe physical phenomena associated with this rich combustion strategy, and the development of a phenomenological model to help interpret the experimental results. The investigation of the reformer consists of experiments in which synthetic exhaust gas is passed through a catalyst testbed, and the reformed products are measured by way of gas chromatography. The combined results of these efforts will serve to refine expectations of the performance of the proposed system as well as begin to address the more practical concerns associated with the operation of the system.

Introduction

Increasing the efficiency of energy systems is an important step towards an overall reduction in anthropogenic CO₂ emissions. For power generation using hydrocarbon fuels, an increase in efficiency results in a decrease in CO₂ emitted per unit of work output. For systems that are currently deployed, the state of the art systems for large-scale (>10 MW) power generation are natural gas combined cycle (NGCC) systems that can achieve efficiencies of approximately 60% on an LHV basis [1]. If this same technology were scaled down to accommodate distributed and transportation-scale generation (100 kW to 10 MW) the efficiencies would drop significantly and would be less cost competitive with other technologies at that scale. Because of this, piston engines and fuel cells tend to occupy this sector of generation. For these types of systems, the current state of the art for deployed systems is limited to below 50% for distributed generation and only slightly higher than 40% for transportation [2-6].

If we look to improve upon these systems, it is important to understand their current limitations. Piston engines are robust devices that can operate using a variety of fuels and can vary load rapidly without large efficiency changes, but they have significant losses due to heat transfer, unutilized exhaust enthalpy, and combustion itself. A previous research effort aimed at improving the efficiency of piston engines showed that they are limited to an exergy efficiency of 60% due in large part to the significant exergy destruction due to combustion [7]. This destruction is explained by the fact that the fuel oxidation step in an internal combustion engine is an unrestrained process in which no work is extracted as the exergy of the resource is reduced. Previous research identified that by coupling work extraction with the exergy reducing step (as is the case with fuel oxidation in a fuel cell), the exergy reduction is restrained by the rate of work extraction and less exergy destruction occurs during the fuel oxidation step [8]. Fuel cells have their limitations too. They have stringent fuel requirements, higher costs, difficulty varying load rapidly, issues with fuel utilization, and the efficiency decreases as load is increased. This implies that there may be promise combining the two to utilize the benefits of both while compensating for their limitations.

There have been previous efforts to implement this mixed combustion/electrochemical strategy for large-scale power generation that have yielded efficiencies surpassing 70% (LHV) [9, 10]. Our goal here is to investigate the prospects of employing this strategy to achieve those efficiency gains at transportation scale. Modeling work performed as part of this research has shown that a system combining an insulated Diesel engine with a solid-oxide fuel cell (SOFC) can achieve efficiencies near 70% (LHV) by reducing the overall reaction-related losses. With this system showing promise, the current research efforts are aimed at assessing the validity of the model assumptions with the hope that further understanding will continue to move this idea towards a realizable system.

Background

To place the progress made into the broader context of increasing the efficiency of transportation-scale piston engines, it is important to discuss the sources of exergy destruction in typical piston engines outlined in the exergy analysis performed by

Johnson and Edwards [7]. Figure 1 shows the results of that exergy analysis for typical spark-ignition and Diesel engines as well as the exergy analysis of three low heat rejection (LHR) Diesel engines. In this graph, the blue “Work” bars correspond to the useful output (and thereby the exergy efficiency) of each engine, and the remainder of the bars correspond to various loss terms. Viewing engines in this way allows us to identify the three main sources of exergy destruction of a typical engine as the loss due to heat transfer out of the engine, the loss due to high temperature exhaust carrying unutilized thermal exergy out of the system, and the loss due to the combustion process. The LHR engines (#3-5) show that the heat transfer and exhaust losses can be reduced by insulating the engine and employing some form of thermal exergy recovery, either through steam injection or a Rankine bottoming cycle. This increases the overall exergy efficiency to just below 60%, a significant increase over the 42% of a standard turbo-charged Diesel.

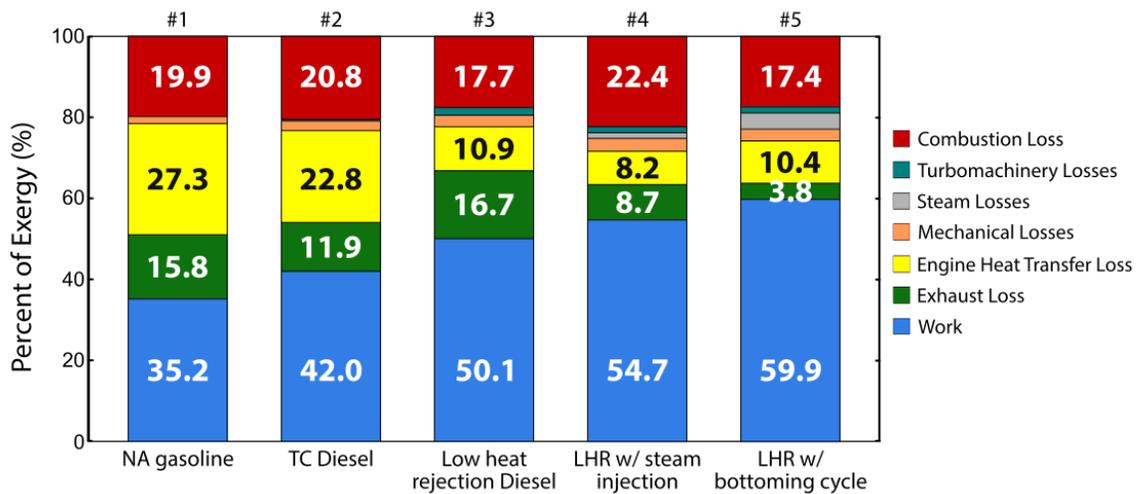


Figure 1: Exergy breakdown of two conventional engines (#1 and #2) and three low-heat-rejection Diesel engines (#3-5). Exergy efficiencies in excess of 60% remain unreachable largely due to the remaining exergy loss from the combustion process (> 17% in all cases) [7].

Within the past year, there have been other efforts aimed at addressing these losses. To name a few, Toyota has developed a new piston bowl geometry with a “thermo swing” coating to reduce convective heat transfer losses in Diesel engines, and researchers at the University of Wisconsin-Madison have investigated a thermochemical recovery strategy that uses the thermal exergy in the exhaust to drive endothermic reforming of Diesel fuel for increased efficiency and enhanced combustion characteristics [11, 12]. While these efforts are useful in exploring other means to address the heat transfer and exhaust losses, they don’t address the combustion loss that is the primary focus of our efforts here. Another outside effort that does aim to address the combustion losses in a similar manner to ours is that of General Electric [13]. Their system runs on natural gas and places the engine downstream of the fuel cell with a small-scale, distributed power generation application in mind. While their intended fuel, system design, and application differ from our research, their quoted efficiencies in the range of

extends into the expansion stroke of the engine cycle where the in-cylinder gas begins to cool and the reactions are less facile. The proposed high-efficiency architecture relies on a low heat rejection strategy in which some of the cylinder surfaces are insulated to allow for the in-cylinder gases to reach a higher temperature at top dead center (TDC) as well as remain at higher temperature through the expansion stroke. Without further experimental investigation, though, it is unclear whether the temperature will remain high enough throughout the combustion process to allow the injected fuel to fully react to its desired gas-phase products.

In order to measure exhaust species concentrations in the rich combustion regime, existing measurement devices in the lab needed to be modified to measure the increased concentrations of CO, H₂, and hydrocarbons above typical engine exhaust. To do so, a dilution system was developed to allow for this increased measurement capability. To dilute the exhaust gas to measure increased concentrations of CO and H₂, the process is relatively straightforward. If the flow rate of the exhaust sample can be determined, an additional stream of N₂ can be added to the sample flow to dilute the concentrations to the desired amount. For hydrocarbons, the process is the similar, but with an added constraint that the sample gas is heated to prevent larger hydrocarbons present in the exhaust from condensing before the measurement device. Since maintaining the high temperature of the heated sample through the dilution system is more difficult, the approach used was to add nitrogen at a known flowrate to the heated sample of a known composition, and then measure the change in analyzer reading to determine the dilution factor. By assuming that the difference in flowrate between the known composition stream and the experimental stream would be small, the experimental stream's composition can be measured on existing equipment with limited uncertainty.

Another challenge encountered in the pursuit of measuring rich combustion products is the measurement of the equivalence ratio itself. In the current experimental setup, the equivalence ratio is measured by a commercial wide-band lambda sensor. Because these sensors are used to measure equivalence ratios around 1.0, though, they are not designed to measure equivalence ratios greater than 1.6. The experimental setup must be modified, then, to measure the desired equivalence ratios out to 2.0 by measuring the flowrates of both the air and the fuel into the system. The measurement of the air can be determined through an orifice designed such that the flow through the orifice is choked and the flowrate depends only on the upstream pressure, which is easily measured by way of a pressure transducer. The fuel flow, however, requires a different approach. One could measure the flowrate directly, but due to the operating principle of a Diesel injector, there is significant bypass flow that would also have to be measured to determine the flowrate of the injected fuel. This would also involve the installation and calibration of flow meters into the current fuel delivery system. A simpler way, then, and the way that was chosen, is to measure the flowrate gravimetrically by measuring the difference in weight of the fuel tank from which the fuel is drawn and into which the return flow returns over a period of steady operation. The rate of change in weight of the fuel tank can then be used to determine the flowrate of the injected fuel.

These two important modifications were necessary before exhaust gas species could be measured at the equivalence ratios of interest. Preliminary data, without these additions, up to an equivalence ratio of approximately 1.5 indicate there will be significant hydrocarbon emissions ($> 10,000$ ppm) for equivalence ratios richer than 1.4 for methanol and ethanol, but with soot values still around the noise floor of the soot analyzer for methanol and a factor of 2 or 3 above current regulation limits for ethanol. Because another ongoing part of this research is to characterize the catalytic reformer's behavior in this regime, it remains to be seen how the presence of significant hydrocarbons in the engine exhaust will affect the performance of the overall system. In the case of ethanol, though, the presence of soot doesn't bode well for the downstream components. It is important, then, to look at other potential methods to reduce the soot concentrations beyond the single injection strategy used in the preliminary exploration.

Soot Mitigation Through Multiple Injection Strategies

In order to overcome the aforementioned soot problems, multiple injection strategies are being investigated as potential soot mitigation tools. Based on other research on multiple injection strategies, we anticipate a factor of two or three reduction in engine-out soot emissions may be possible. The injection strategies include pilot, split-main, and post injections. Each type of injection offers different features to help decrease soot emissions. Pilot injections increase in-cylinder turbulence to enhance mixing for the main injection. In split-main injections, the second injection enters the slipstream of the first, allowing it to penetrate faster and increasing turbulent mixing. Finally, post injections can mitigate engine out soot emissions through enhanced mixing, increased in-cylinder temperature, and limiting the "jet replenishment" by decreasing the injection duration of one injection event. Increased temperature creates the desired conditions for soot oxidation, and enhanced mixing and the jet replenishment increase the air utilization.

To achieve multiple injections within a single engine cycle, a fast acting fuel injector is required. Bosch CRI 3.0 Piezo Acting Injector provides the desired rapid response for multiple injections. To provide a better understanding of the piezo injector operation, a dynamic model was developed. Figure 3 shows an example of the fuel injector model result that includes the injector lift profile and the pressure dynamics during the injection.

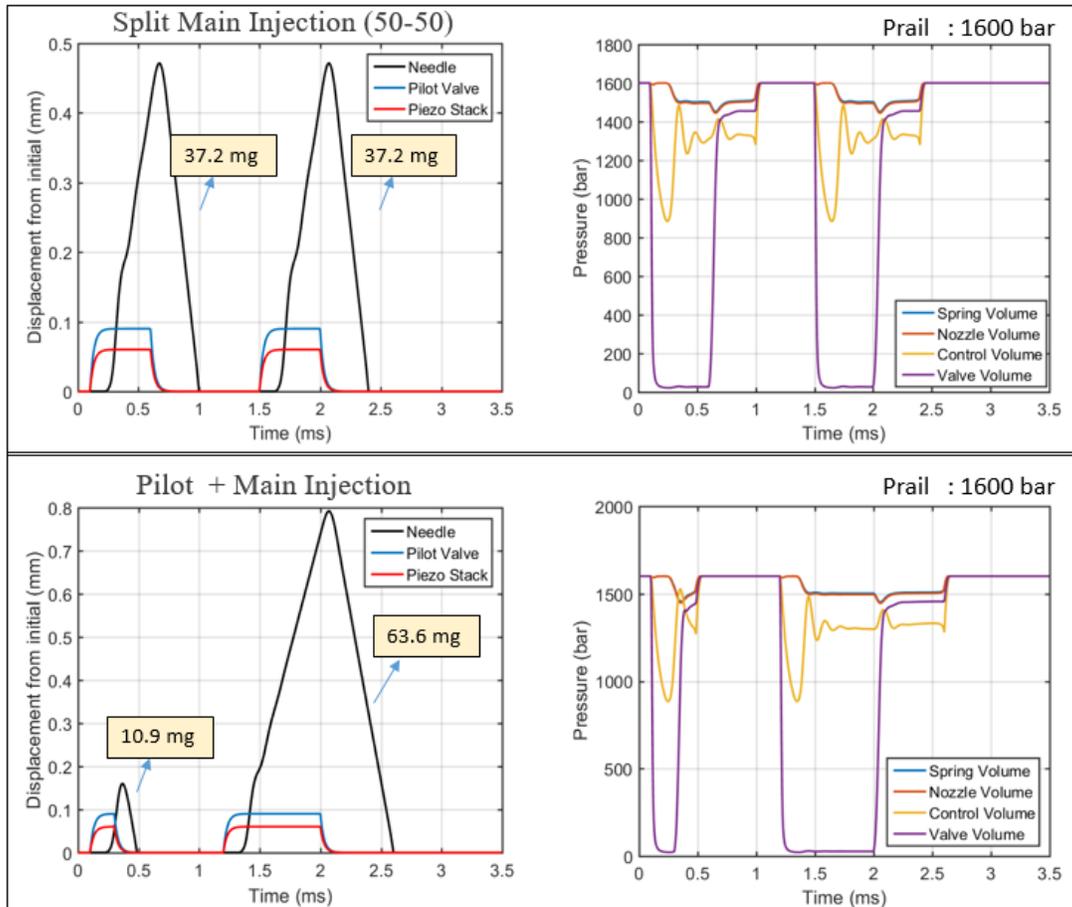


Figure 3: Injection model results for a split-main injection (50-50) and a pilot and main injection

The model's performance will need to be compared with that of a working injector for validation purposes. To accomplish this, an injector driver circuit is being developed. The challenge with the driver circuit is to obtain the shortest dwell between two injection events. The current aim is to bring the dwell time to around $80 \mu\text{s}$, which corresponds to roughly 1 crank angle degree (CAD) at an engine speed of 2000 RPM. After achieving the desired injection characteristics, different injection strategies will be investigated through optical access experiments in our extreme compression device.

Phenomenological Model Development

Models, both conceptual and numerical, can be useful tools in interpreting experimental results. A typical conceptual model of Diesel-style combustion splits the exothermicity associated with the combustion process into phases, beginning with an initial ignition delay period and followed by a premixed combustion phase in which the fuel and air that have been premixed during the ignition delay period autoignite. Following this phase, there is a mixing-controlled combustion phase, during which the rate of turbulent mixing of the fuel and air limits the rate of exothermicity. This mixing controlled phase decreases in its rate of exothermicity as it extends into the expansion stroke and the in-cylinder gases begin to cool, ultimately ending when the majority of the

fuel has been reacted or the chemical kinetics have become sufficiently slow to render the reactions effectively frozen.

In the case of the combustion strategy employed in the high-temperature system under investigation here, it is anticipated that the combustion process will have some key differences. First, due to the higher in-cylinder temperatures, the ignition delay period should be reduced as the reactions will be more facile. This won't allow for as much time for premixing fuel and air, and should ultimately lead to a reduction in the fraction of total exothermicity attributed to the premixed combustion phase. This, in addition to the fact that the injection durations will need to be significantly longer to deliver all of the fuel required to reach the desired rich equivalence ratios, will lead to a much more significant portion of the exothermicity occurring in the mixing-controlled combustion phase than typical Diesel-style combustion. This difference not only requires an adaptation of the typical conceptual model used to describe Diesel-style combustion, but also motivates the need for other numerical tools that can be used to interpret the effects of the relevant phenomena for combustion in this regime.

Models used to describe Diesel-style combustion focus on many different aspects of the overall combustion process, ranging from the initial droplet formation and vaporization, to the mixing and entrainment rates of air into the fuel jet, to the exothermicity associated with the chemical reactions that occur throughout the process. The key areas of interest for our investigation, though, are the energetics associated with combustion and the exhaust gas species concentrations. These are the pieces relevant to the proposed overall system and are the purpose of the experimental investigation outlined above. In developing a numerical model to help interpret the experimental results, then, it is important to account for the major physical phenomena that impact these performance metrics. Because it is anticipated that the mixing-controlled phase will constitute the majority of the combustion event, this has been the primary focus in the development of the phenomenological model used to describe combustion in this regime.

The new phenomenological model developed for this application conceptually builds off a previous model developed by Broadwell and Lutz that modeled combustion as a quasi-steady fuel jet represented by two coupled reactors [15]. Their model has been used previously to study NO_x and soot formation and assumes a quasi-steady process with constant pressure and chemical composition of the surrounding gas [16, 17]. The key aspect of their model that is utilized in the new model is the representation of the mixing-controlled combustion phase as two coupled reactors, one representing the flame sheet where reactions proceed quickly relative to fluid dynamics and the other representing the core as a well-mixed, locally-homogeneous region where reactions proceed according to chemical kinetics. The models differ in that the newly developed model is transient to account for the varying in-cylinder state over the duration of the combustion process and is spatially confined to allow for the reactions to drive pressure changes in the in-cylinder state. Doing so will enable the model to investigate the effects of the interactions between the fluid dynamics, chemical kinetics, and energetics on the work output via the pressure trace as well as the ultimate exhaust gas species concentrations.

Figure 4 shows a graphical representation of the new phenomenological model's mixing-controlled combustion phase. The model tracks n two-stage reactor pairs as they travel down the injection axis and evolve in time. Doing so allows the last bit of fuel introduced to experience a different in-cylinder state than the first bit of fuel to investigate the effects the changing cylinder state may have on the chemical composition of these fuel parcels as they are mixed with air and allowed to react. The reactor pairs interact with the ambient gas via an experimentally derived entrainment rate, and interact with each other and the ambient by expanding or compressing to accommodate the overall volume constraint and a common in-cylinder pressure among all modeled zones.

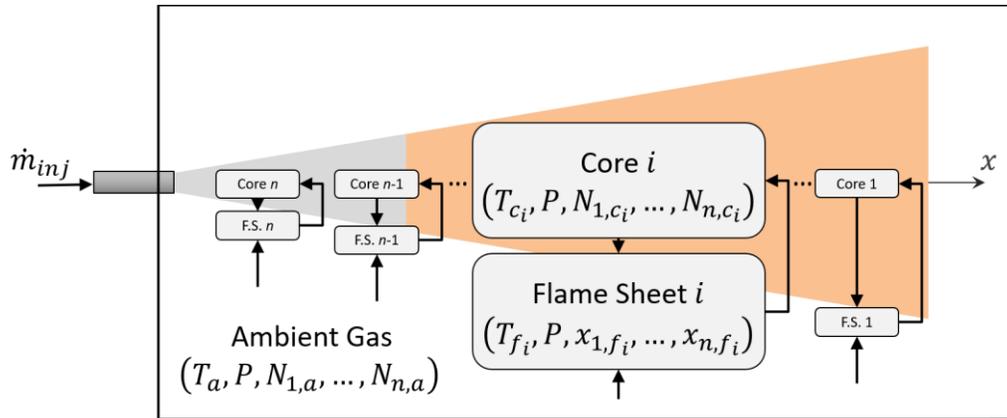


Figure 4: New phenomenological model developed for interpreting experimental results

Before the validity of this approach can be assessed, the processes that bridge the gap between the free-jet, mixing-controlled combustion phase and the late-stage, mixing-controlled combustion phase need to be represented in some way. In order to do that, however, the physical phenomena associated with the later mixing-controlled combustion phase, in which the jet is interacting with the wall and it is no longer accurately represented as a free jet, must be observed in the rich regime. Typically, the wall interacting portion of Diesel-style combustion occurs towards the end of injection, and makes up a relatively small portion of the overall combustion process. As mentioned before, though, in the rich regime, injection durations become significantly longer, and the wall-interacting portion constitutes a much more significant part of the overall combustion process. To better understand this period, optical access experiments on a single-cylinder research engine designed to withstand full-load Diesel combustion pressures will be performed before concluding the model development. Those experiments are forthcoming, and with the insights gained there, the model can be finalized, and the validity of the model can be assessed using the measurements made during the rich combustion experiments outlined above.

Catalytic Reforming Investigation

Finally, the reforming stage of the system is being investigated to determine if the modeling assumptions remain valid despite operating outside of typical operating environments. Steam reforming in the presence of exhaust gas has been explored

previously, but small differences in operating conditions can have large effects in catalytic systems. Therefore, an experimental catalytic reactor system was developed to characterize the products of reforming under the conditions in used in the model. This includes reactant mixtures with no fuel or water added as well as mixtures with large fuel and water additions. In addition, the experiment will explore reforming up to 5 bar, the modeled system pressure, to ensure that any pressure-related affects are accounted for.

The catalytic reactor system consists of a reactant mixture delivery system, a heterogeneous catalytic reactor, and a gas chromatography (GC) system to determine the reformat species concentrations. The reactant mixture delivery system uses mass flow controllers for the gas phase species and a syringe pump and evaporator for liquid species.

The GC was designed to measure the concentration of the reformat species, with the exception of soot. The GC contains two separate analytical “lines” that are designed for measuring different species. The first uses a capillary column and an FID capable of measuring hydrocarbon and alcohol species, while the other uses multiple packed columns, a valve program, methanizer, and a TCD/FID combination to separate and measure the “fixed” gases (typically this refers to CO₂, N₂, O₂, H₂, CO) as well small hydrocarbons such as methane and ethane.

Progress

Our approach towards increasing the efficiency of transportation scale systems aims to reduce greenhouse gas emissions by reducing the fuel required to produce one unit of work, thereby reducing the CO₂ emissions associated with that one unit of work. This is illustrated graphically in Figure 5 below. A given fuel has an associated work potential and an associated carbon content. Our goal of reducing greenhouse gas emissions can be thought of as moving to the left on this graph, and our means of accomplishing this, without using carbon capture strategies, would be to either use fuels with a lower carbon to exergy ratio (e.g. using natural gas rather than gasoline) or increase the efficiency of systems that use a given fuel.

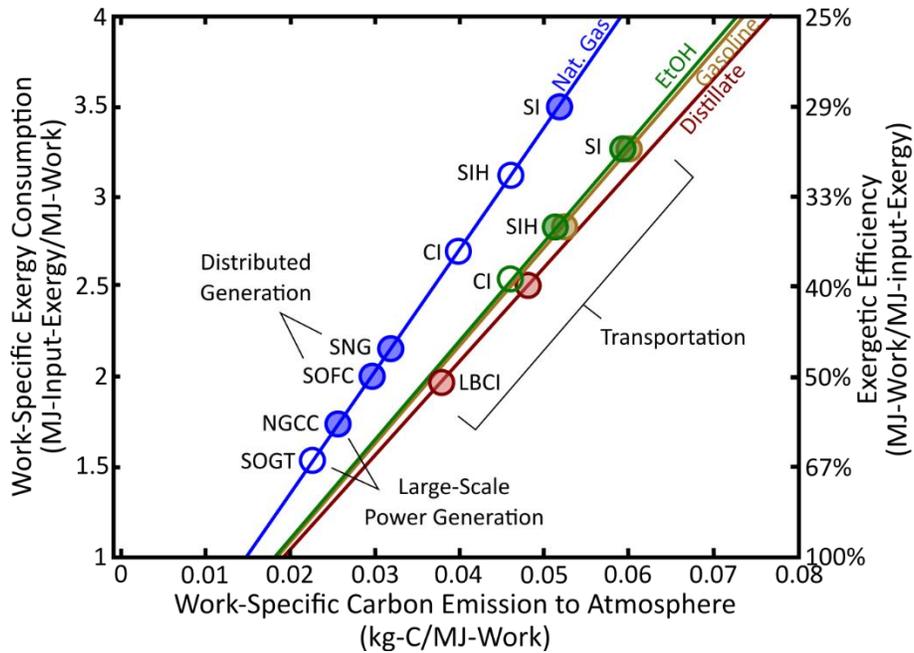


Figure 5: Work-specific exergy consumption, exergy efficiency, and work-specific carbon emissions for energy systems currently deployed (filled circles) and under development (unfilled circles) [1-6, 9, 18-21].

Our proposed system, if successful, could dramatically reduce the CO₂ emissions associated with transportation. We envision this system as being well suited for the heavy-duty transportation sector, where the engine could provide the power on demand when required and the fuel cell could provide a sustained, high efficiency power output for lower load points. If we compare our most efficient system at 67.5% exergy efficiency to a turbo-charged diesel operating at 42% exergy efficiency, it amounts to a reduction in work-specific carbon emission to the atmosphere of approximately 35%. The 2016 International Energy Outlook identified that transportation accounted for 25% of the world energy demand in 2012 and increasing with a projected annual average rate of 1.4% from 2012 to 2040 for their reference case [22]. A 35% reduction in CO₂ emissions associated with this sector would have a significant impact on global greenhouse gas emissions.

Future Plans

Our efforts over the past year have placed us in a position to complete our research goal in the near future. With the increased measurement capabilities that have been put into place, we are well positioned to characterize the rich combustion regime in terms of its performance and emissions. Doing so will allow us to test the assumptions made in the development of our system model and address the concerns with using this combustion strategy as a fuel reforming step in the overall system. With the development of the phenomenological model, we can better understand the influence of the physical processes associated with this combustion strategy on the emissions and performance of the engine by using it to interpret the rich combustion experimental results. This knowledge will aid in adjusting the combustion strategy should this base case prove to be

somewhat limited in its application. The experimental efforts focused on multiple injection strategies represents one of the possible adjustments that could be made to reduce the soot emissions for ethanol or higher hydrocarbons. The progress made there on the modeling front allows for a better understanding of the dynamics of the injector that is critical to a multiple injection strategy. Finally, the catalytic experimental setup will enable us to explore the range of acceptable feed gas compositions as they relate to hydrogen output as well as catalyst performance and degradation.

In the coming months, rich combustion experiments will be performed in our optical-access research engine to observe the phenomena associated with very rich, DI-CI combustion. This insight will be used to finish development on a phenomenological model intended as an interpretive tool for future combustion experiments. Next, rich combustion experiments will be performed in our other single-cylinder research engine that will serve as a better representation of expected performance in an LHR engine. Using the phenomenological model, the influence of physical processes that are a part the overall combustion process will be investigated. In parallel to those efforts, the multiple injection strategy will be experimentally explored in our extreme compression device by performing multiple injections and assessing their viability for soot mitigation. This will be accomplished by comparing the luminosity observed during the multiple injections to that which has been observed for methanol, a fuel that has been shown in previous experiments to produce no appreciable engine-out soot emissions. The third parallel research effort will perform characterization experiments for the catalyst performance in this regime. These experiments will consist of feeding tailored feed gas compositions that are intended to be representative of the feed gas anticipated in our application through the catalyst bed and measuring the composition of the output gas by way of gas chromatography. The combination of all of these efforts will extend our knowledge of the proposed system as well as the overall mixed combustion/electrochemical space. The result will be a relatively robust understanding of the prospects of using a mixed combustion/electrochemical strategy to address our overall goal of achieving efficiencies above 60% for transportation-scale power generation.

Publications and Presentations

Publications

1. J. R. Fyffe et al. [Mixed combustion–electrochemical energy conversion for high-efficiency, transportation-scale engines](#). *Int. J. of Engine Res.*, 1468087416665936, Mar. 2016.

Presentations

1. M. A. Donohue, “Mixed combustion/electrochemical energy conversion for high-efficiency, transportation-scale engines,” technical presentation at *ASME International Mechanical Engineering Congress & Exposition, Phoenix, AZ, USA, November 11-17, 2016*.

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