Development of Low-Irreversibility Engines

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This project aims to implement the concept of low-irreversibility combustion in reactive engines to improve efficiency. Section 1 explains the thermodynamic concepts of maximum available work, entropy, and irreversibility generated by the combustion process, as well as their relevance to engine efficiency. The novel concept of low-irreversibility combustion is introduced. Section 2 discusses dilution of the fuel-air mixture with residual gas as a strategy to slow down the kinetics of combustion. Section 3 presents preliminary results of implementing such a dilution scheme in homogeneous charge compression ignition (HCCI) combustion of hydrogen. Section 4 describes the preliminary design of a test facility for the study of low-irreversibility combustion in steady flow. And Section 5 outlines future work and the direction of the research. Because hydrogen is a simple fuel with a well-understood combustion reaction mechanism it is used in all modeling and experimental studies reported here. Preliminary studies using a hydrocarbon fuel (propane) have also been conducted and will be reported at a future date.

1. Background

Combustion engines release chemical energy contained in an air-fuel mixture by burning it. The resulting hot products serve as the working fluid whose sensible energy is converted to useful mechanical work. We refer to engines that execute the energy conversion process continuously as “steady-flow” engines; gas turbine engines are included in this category. In contrast, piston engines are “batch-flow” engines that process the charge in a sequence of discrete events.

Once initiated, combustion in a conventional engine is rapid and unconstrained. The chemical reaction is confined to a very thin zone – the flame front – that propagates until all reactants are consumed. The exothermic process is rate-limited by local diffusive and convective transport of energy and species at the flame front. The efficiency of energy conversion by such a process can be quantified using thermodynamics principles.

We first analyze the gas turbine engine, a steady-flow device. In this engine, atmospheric air is compressed to high pressure and mixed with fuel. The reactant mixture is then ignited, and the resulting combustion products at high temperature are expanded through the turbine to develop work. The Brayton model is an idealization of the gas turbine cycle.

Figure 1 shows the result of an ideal Brayton cycle analysis on a Mollier (enthalpy h versus entropy s) diagram. The net work developed by the engine is given by the enthalpy difference between the initial reactant and final product mixtures, both at atmospheric pressure. A theoretical “isentropic” chemical reaction (1 – 4s) would yield the maximum work available, w_{MAX}. State-of-the-art gas turbine combustors, on the other hand, operate adiabatically with minimal pressure loss. The rapid combustion process (2 – 3) leads to maximum rise in temperature (up to the adiabatic flame temperature) and high entropy production. As a result, the net work, w_{NET} actually developed by the engine is less than w_{MAX}; the difference is the irreversibility (or lost work), i due to combustion. The ratio of w_{NET} to w_{MAX}, a form of second law efficiency, is therefore a sensible measure of how well the engine utilizes its fuel.

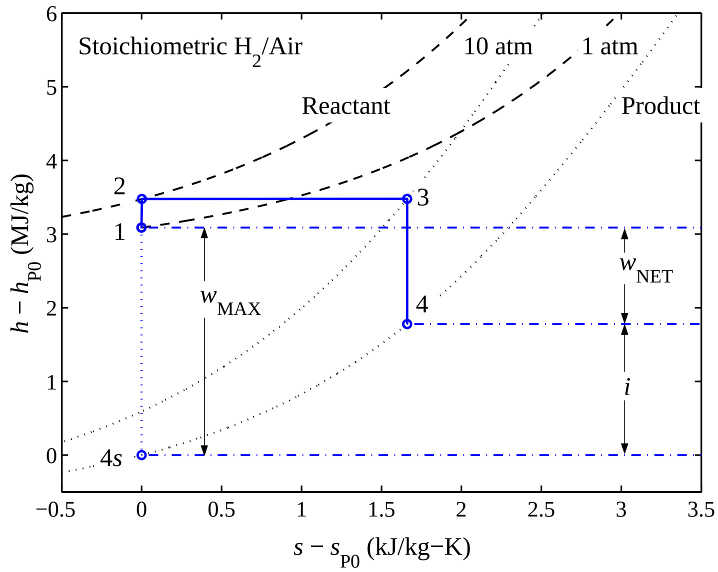

Figure 1: *h* - *s* diagram for an ideal Brayton cycle (steady flow engine).

The piston engine can be similarly modeled and analyzed. The Otto cycle is a simple model of how a piston engine operates: The reactant gas mixture is compressed and then ignited while the piston is at top dead center (TDC). The adiabatic combustion products are expanded back to the original volume and thereby produce mechanical work.

The total internal energy *u* versus entropy *s* diagram (Fig. 2) shows the result of an ideal Otto cycle analysis. w_{MAX} is given by a theoretical "isentropic" chemical reaction from reactants to products at the same specific volume (1 – 4s). Again, adiabatic, constant-volume combustion at top dead center generates entropy and irreversibility, so only a fraction of maximum available energy is converted to useful work.

The concept of low-irreversibility combustion stems from the realization that, from the second law standpoint, there is opportunity, currently unexploited, to extract additional useful work during the combustion process. Instead of allowing the reactant mixture to combust rapidly without constraint, a low-irreversibility engine would harness useful work from chemical energy released *as* combustion is occurring. Figure 2 illustrates the potential efficiency improvement based on this concept. A 20% reduction in entropy generated during combustion near TDC (due to work extraction), for instance (2 – 4*), would increase w_{NET} by 30%.

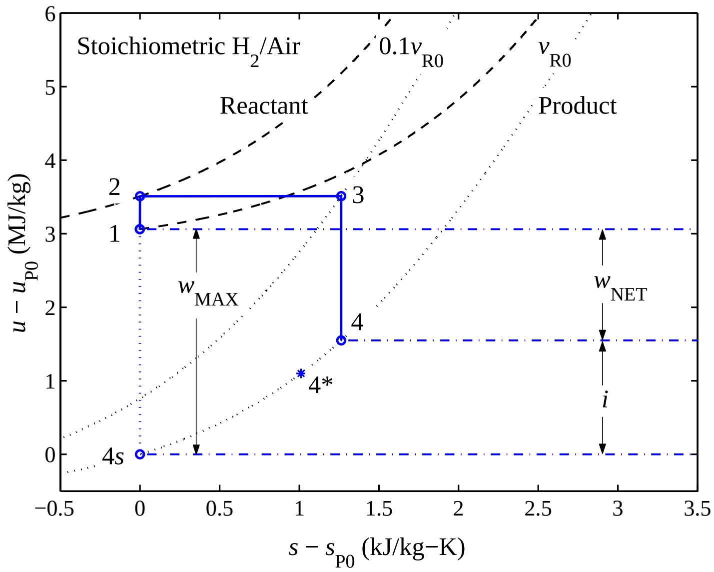

Figure 2: *u* - *s* diagram for an ideal Otto cycle (batch flow engine).

This project is studying possible processes (e.g., from 2 to 4* in Figure 2) that can achieve such entropy and irreversibility reductions. Implementation of this combustion concept requires the chemical reaction be controllable. A potential method to realize that through dilution of reactant mixture with hot exhaust gases is discussed in Sections 2 and 3. Additionally, careful design of the work extraction process, aided by intelligent control strategies, will likely be necessary to drive the combustion process to completion and avoid quenching.

2. Dilution for Controlling Combustion Kinetics

Conventional combustion is characterized by an intense, localized reaction zone with steep spatial gradients of temperature and species concentration. The process is transport-dominated and not amenable to automatic control schemes. The mode of combustion can be altered to be rate-limited by chemical kinetics by diluting the fresh fuel/air mixture with re-inducted exhaust gases. This dilution technique has been implemented successfully in piston engines running in homogeneous charge compression ignition (HCCI) combustion mode.

The hot exhaust raises the sensible energy content (and thus temperature) of the mixture to sustain the reaction and avoid quenching. At the same time, the temperature rise during combustion is moderated due to the overall lower chemical energy content of the dilute reactant mixture. A well-mixed, homogeneous charge can autoignite uniformly, eliminating the difficulty of controlling a process driven by strong spatial gradients.

On the other hand, the time scale of the combustion process also affects its controllability. Homogeneous combustion that does not depend on flame propagation has shorter combustion duration, and hence imposes higher bandwidth requirement on the controller.

An analysis has been performed to study the effects on combustion duration due to variations in dilute mixture temperature and dilution fraction. The calculations are done using Cantera, an open-source program for chemical kinetics and thermodynamic simulations, in conjunction with the suite of ODE solvers in MATLAB. The non-carbon subset of the GRI-Mech 3.0 combustion reaction mechanism and its associated thermochemical data are used in the analysis.

The sequence of processes analyzed starts with the compression stroke of a reciprocating engine (geometric compression ratio, $r_C = 10$, ratio of connecting rod length to crank radius = 5.52) operating at 1800 RPM. The process is assumed to be adiabatic. Under these conditions, a stoichiometric mixture of hydrogen/air diluted by 50% (by mass) of combustion products (water and nitrogen) initially at 500K, 1 atm would autoignite just before TDC.

For mixtures with higher dilution, the compression stroke raises the mixture temperature and starts the chemical reactions by building a pool of reactive radical species. However, a power stroke *immediately* following the compression stroke would quench the combustion reaction. Instead, the "mildly combusting" mixture is held at constant volume until peak pressure is reached, at which point the power stroke resumes; the mixture is allowed to expand adiabatically as the piston returns to BDC.

Figure 3 is a representative pressure trace generated from the simulation. We define ignition delay, t_{IGN} as time for 5% pressure rise from the end of the compression stroke, and ignition duration, t_{DUR} as the time for the pressure to rise from 5% to 95% of the pressure rise during the constant-volume combustion region. While the finite-time constant volume combustion process clearly defies the geometric constraints of a reciprocating engine, it provides a quantitative measure of the chemical time scale during which the process must be controlled.

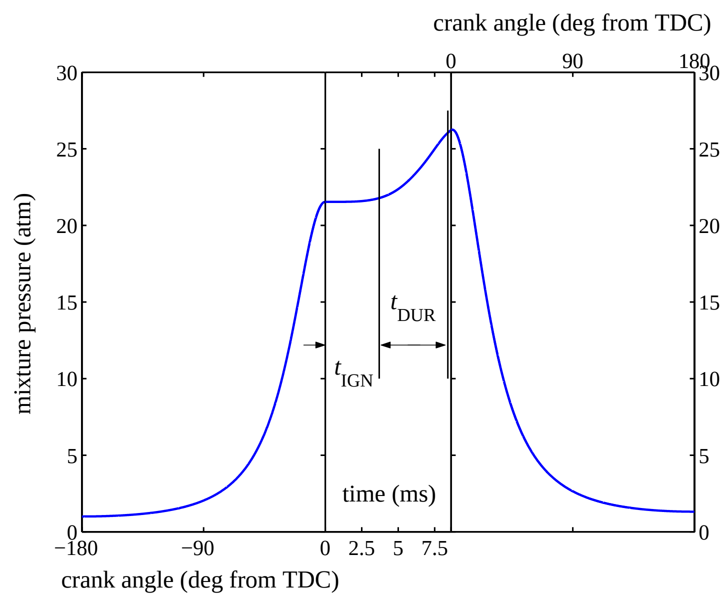

Figure 3: Mixture pressure as a function of crank angle / time for the simulated homogeneous combustion process. The mixture is stoichiometric hydrogen/air diluted with 9 times (by mass) combustion products (water/nitrogen), initially at 500K.

Figures 4 and 5 compare the ignition delays and durations for reactant mixtures of varying dilution factor (defined as the ratio of mass of exhaust re-inducted to total mass of the diluted mixture) and initial temperatures (at the start of compression stroke). As a matter of comparison, an engine running at 1800 rpm would move approximately 10 crank angle degrees in 1 millisecond.

The results show high sensitivity of the combustion process to mixture temperature. This is to be expected since the rate of chemical kinetics scales exponentially with reactant mixture temperature. The results also show potential, as well as challenges, for control of the homogeneous combustion process. After the compression stroke, it would take another millisecond to ignite a 75% dilution mixture initially at 500 K. This time scale may be amenable to a control schemes based on cylinder volume. Upon ignition, however, the mixture takes less than a millisecond to complete combustion. Lowering the initial charge temperature or increasing the dilution factor would help slow down the reaction kinetics.

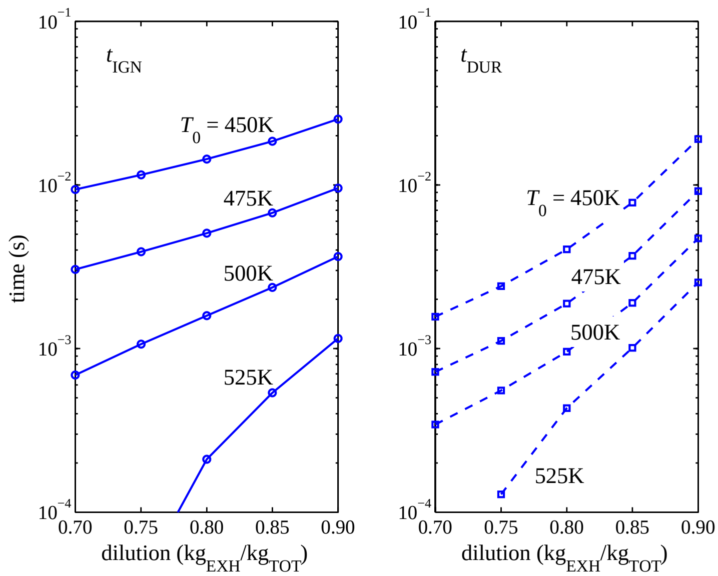

Figure 4: Ignition delay and combustion duration as a function of dilution factor, for varying initial mixture temperatures.

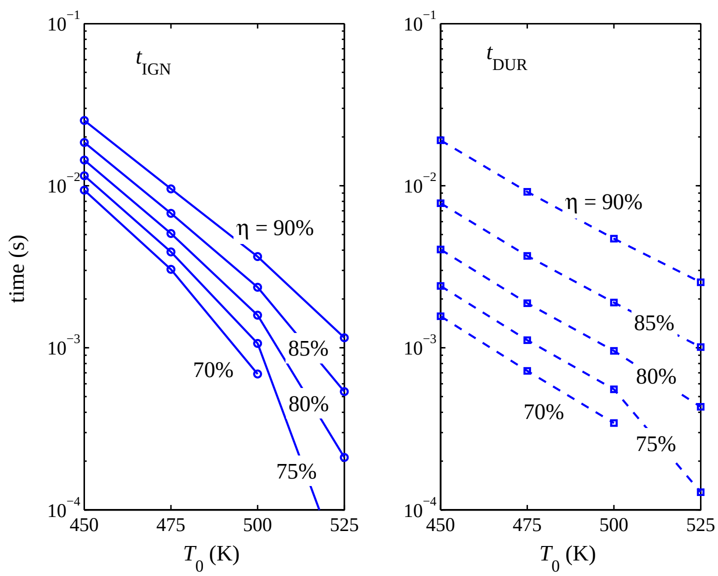

Figure 5: Ignition delay and combustion duration as a function of initial mixture temperature, for varying degree of dilution.

3. Hydrogen HCCI implementation

Figure 6 shows the schematic drawing of the homogeneous charge compression ignition (HCCI) engine, a piston engine coupled with a special valve system, studied in this project. HCCI is implemented by re-inducting hot exhaust gases on the intake stroke, which serves to both dilute and preheat the fresh charge. The preheating adds sufficient energy so that autoignition occurs during compression.

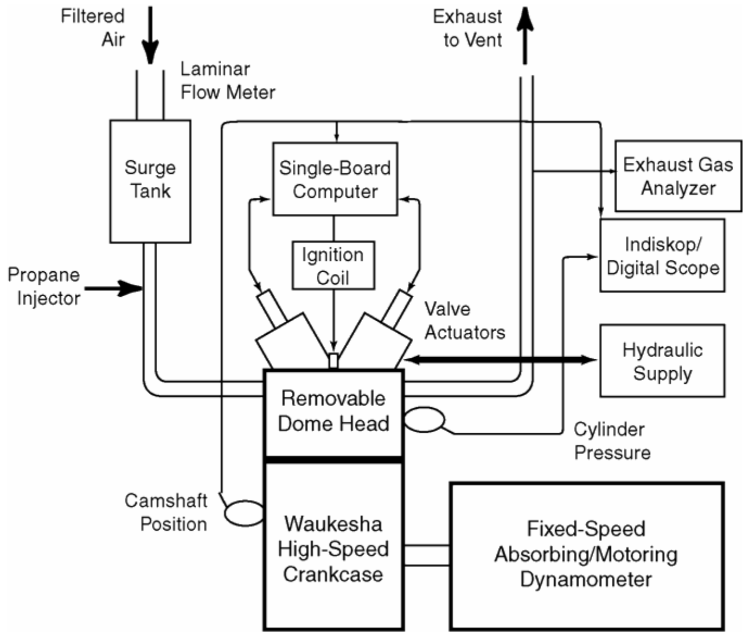

Figure 6: Schematic diagram of Stanford HCCI engine.

In order to re-induct exhaust gas we have implemented arbitrary control of valve motion. A single-board computer controls a spool valve which in turn regulates the flow of high-pressure hydraulic fluid that powers the valves. Currently, we switch to HCCI by holding the exhaust valve open during the intake stroke. The valve system is mounted to a single-cylinder Waukesha engine that allows compression ratio to be adjusted during operation.

A necessary step in achieving low irreversibility combustion is first being able to operate in the HCCI combustion mode using hydrogen. We recently demonstrated hydrogen HCCI for the first time, using the setup described above. We are able to repeatably transition from spark-ignited (SI) operation to HCCI, and can then hold stable HCCI indefinitely. Figure 7 shows a cycle-averaged pressure trace from our first stable run of hydrogen HCCI.

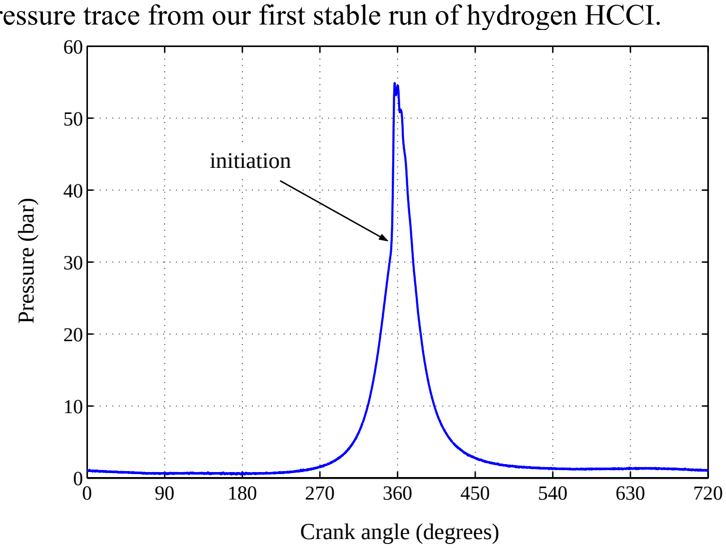

Figure 7: Cycle averaged pressure trace from hydrogen HCCI implementation.

4. Design of Steady-Flow, Low-Irreversibility Combustor

We have also begun preliminary design work on creating a steady flow version of a low irreversibility engine. Such a device could potentially allow us greater freedom in coupling energy extraction to chemical energy release during combustion. The basic processes are the same as for the batch version: dilution, energy addition, autoignition, and energy extraction during combustion.

In designing the test facility, we want to consider a wide range of possibilities. Dilution and preheating are again accomplished using hot combustion products, but the production of these gases is decoupled from the primary combustor in a separate vitiation gas generator. There are three required energy exchanges: lowering the vitiation gas temperature, raising the mixed products and reactants to the autoignition temperature, and extracting energy during low irreversibility combustion. Three choices are possible for each: heat transfer, work, and exchange between enthalpy and kinetic energy. Work would require turbomachinery, which is too complicated and inflexible for our first efforts. Calculations indicate that using kinetic energy for cooling and then ignition would require a supersonic mixing chamber, which is not yet well understood. Heat transfer is undesirable for the final energy extraction because it involves strong spatial gradients. Thus we are left with the choices indicated in Figure 8.

Probable choices for specific components are as follows. A liquid-fueled, swirled, diffusion-flame combustor would be used for the vitiated gas generator. For a 50 kW combustor, both of the first two energy exchanges would be on the order of 30 kW. Phase change cooling seems to be the simplest method to reach that power level for the cooling stage. For the heating stage, molybdenum disilicide ($MoSi_2$) high-temperature heating elements are capable of providing the required power and homogeneity. An adjustable supersonic nozzle, while not trivial, seems to be the simplest choice for extracting energy during the final combustion process.

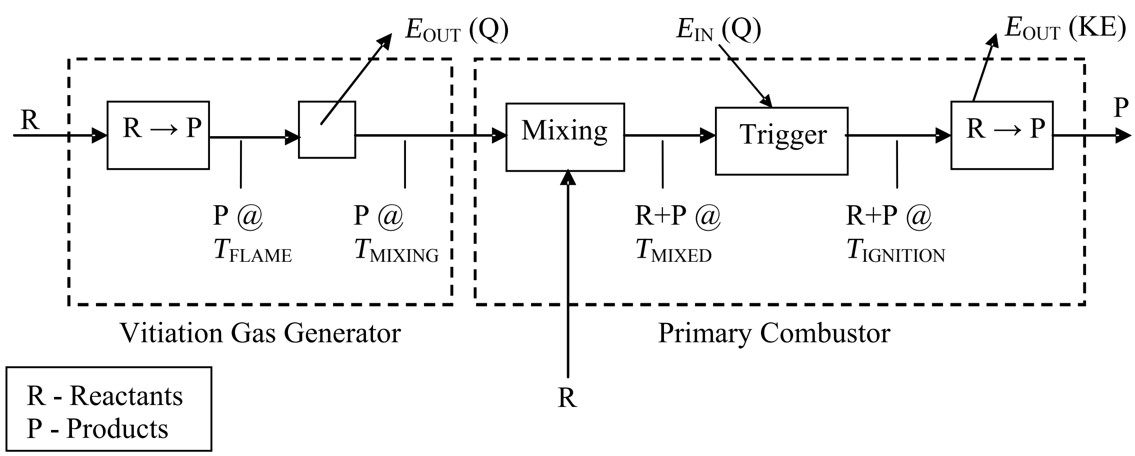

Figure 8: Conceptual design of a low-irreversibility steady flow engine.

5. Future Work

Current research efforts include optimization of work extraction process during low-irreversibility combustion and design of the steady flow low-irreversibility engine. Implementation as well as mapping of hydrogen HCCI performance and emissions – a prerequisite for operation as a low-irreversibility piston engine – are also ongoing.

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