II Advanced Combustion and Emission Control Research for High-Efficiency Engines

II.1 Stretch Efficiency in Combustion Engines with Implications of New Combustion Regimes

Ron Graves (Primary Contact), Stuart Daw, James Conklin, Kalyana Chakravarthy
Oak Ridge National Laboratory
NTRC Site
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager: Kevin Stork

Subcontractors:
University of Wisconsin, Madison, Wisconsin (Prof. David Foster, Mr. Ben Druecke, Prof. Sandy Klein)
Texas A&M University, College Station, Texas (Prof. Jerry Caton, Mr. Praveen Chavannavar)

Objectives

- Analyze and define specific pathways to improve the energy conversion efficiency of internal combustion engines from nominally 40% to as high as 60%, with emphasis on opportunities afforded by new low-temperature combustion regimes.
- Establish proof of principle of the pathways to stretch efficiency.

Approach

- Use literature study to reevaluate prior work on improving engine efficiency.
- Exercise appropriate engine models to define the greatest opportunities for further advancement.
- Develop improvements to those models as needed to address the features of low-temperature combustion.
- Conduct availability (exergy) analyses using the Second Law of Thermodynamics as well as the First Law to study where the large losses inherent in conventional combustion lie.
- Design and conduct proof-of-principle experiments.

Accomplishments

- Began developing in-cylinder phenomenological models for simulating the efficiency effects of low-temperature combustion modes on thermodynamic availability.
- Collaborated with Texas A&M in developing and applying a protocol for using experimental engine data to analyze the major exergy losses during conventional and low-temperature combustion.
- Delivered presentation at the 9th International Conference on Present and Future Engines for Automobiles in San Antonio, May 29-June 2, 2005, that summarized engine loss mechanisms and recommended research paths.
- Demonstrated in collaboration with the University of Wisconsin that closely matched work extraction and combustion as well as all types of homogeneous charge combustion do not offer any significant reduction in inherent combustion irreversibility.

- Demonstrated in collaboration with Texas A&M that smaller-molecule fuels such as hydrogen and methane have inherently lower combustion irreversibility than conventional gasoline and diesel fuels.
- Demonstrated with idealized global engine simulations that any reductions in combustion irreversibility will inevitably lead to hotter exhaust and the need for multi-stage work extraction (i.e., cycle compounding).
- Identified potential inefficiencies in current methods for handling exhaust gas recirculation (EGR) and determined that reconfiguring EGR heat exchangers might yield increased efficiencies of a few percent.
- Continued documentation of two alternative pathways to mitigate the losses of thermodynamic availability (exergy) from traditional flames.

Future Directions

- Continue analyses of data from advanced combustion experiments to determine efficiency implications and appropriate ways to model exergy losses under different operating modes.
- Continue to evaluate ways to reduce irreversibilities in current EGR handling.
- Continue to explore better ways for recuperating heat and extracting work from higher-temperature exhaust.
- Continue to identify ways in which the potentially lower wall heat loss from low-temperature combustion can be exploited for higher efficiency.
- Continue exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses.

Introduction

The best approach for improving engine efficiency is to understand the causes of losses, then develop ways to mitigate them. Numerous studies over the past 30 years have quantified the thermodynamics of engines. A representative distribution of the fuel energy losses as they are currently estimated is shown in Figure 1 [1]. Here we utilize a thermodynamic property known as availability (or exergy) to show how fuel energy is ultimately transformed. Because availability measures the fraction of the original fuel energy that can be converted into useful work, it gives deeper insights into the loss mechanisms than simple energy balances.

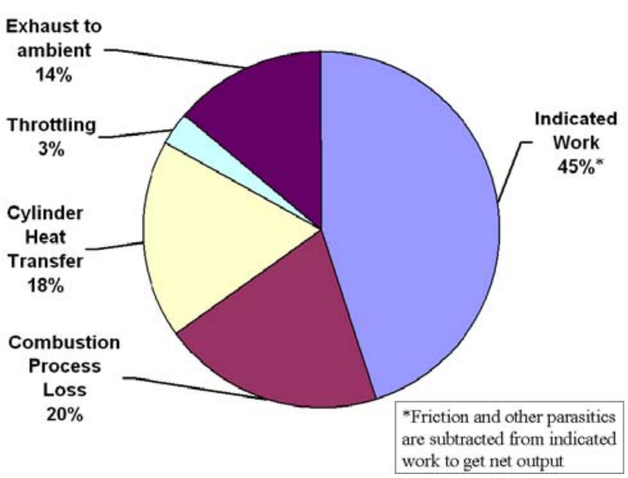

Figure 1. Typical Distribution of Fuel Availability at Full Load for a Simulated Truck Diesel Engine (from [1])

In conventional engines, the largest efficiency losses (approximately 20%) occur in the combustion process itself and are difficult to mitigate. Such losses are not due to unburned fuel, which is a relatively small loss, but they are instead due to the generation of thermodynamic entropy by the unrestrained combustion reactions. The net effect is to divert some of the fuel energy into molecular motion and heat. This diverted energy becomes unavailable to produce useful work according to the Second Law of Thermodynamics. Simple energy balances, which reflect the First Law of Thermodynamics, don't distinguish between available energy (energy that can produce work) and unavailable energy (energy that can only make heat). In principle, it is this entropy-generating characteristic of unrestrained chemical reactions that gives fuel cells their theoretical advantage over

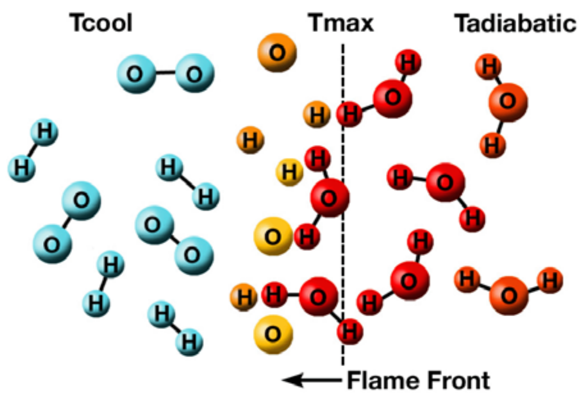

Figure 2. Schematic depiction of entropy generation in a hydrogen flame front. Extremely energetic product molecules dissipate their energy in collisions with surrounding molecules having much lower energy.

existing combustion engines. However, as we discuss below, it is theoretically possible to carry out combustion reactions in a more restrained way that produces less entropy and preserves more of the original fuel energy for work.

Typically, processes that generate entropy are referred to as thermodynamically irreversible. Detailed analyses of the irreversibility of unrestrained combustion have shown that it comes mostly from 'internal heat transfer' between the products (exhaust gases) and reactants (fuel and air). Such heat transfer is inevitable in both pre-mixed and diffusion flames, where highly energetic product molecules are free to exchange energy with unreacted fuel and air [2]. Since these molecules have large energy (i.e., temperature) differences, considerable entropy is generated when they interact. This entropy generation process is depicted schematically in Figure 2.

In general, combustion irreversibility is mitigated if the reactions take place nearer chemical equilibrium. This can be accomplished when the reactants are preheated reversibly (slowly, with small temperature gradients) such that they are brought closer to the temperature of the products. We recently published an article describing a theoretical generic isobaric combustion process that could accomplish this near-equilibrium preheating and reaction [3]. It appears that some aspects of reversible preheating may also be present in combustion processes like homogeneous charge compression ignition (HCCI) or low-temperature combustion (LTC). Thus, there has been interest in investigating the combustion reversibility of these advanced combustion modes.

Approach

Through analysis and experiment, we are investigating the types of internal engine combustion processes that can reduce combustion availability destruction. Last year's extensive literature review continues to be expanded, with emphasis on Second Law analyses of engine processes. We are combining in-house thermodynamics codes with phenomenological in-cylinder combustion models and commercial engine/system models such as Ricardo WAVE to perform availability balances for both hypothetical and experimental engine configurations and combustion modes. University partners are also collaborating with us in these analyses.

Results

In this fiscal year we completed development of computational physical property subroutines for engine availability balances. These subroutines were combined with in-cylinder combustion models to simulate the efficiency of low-temperature combustion modes. The latter models are phenomenological in construction and involve very simplified descriptions of the combustion reaction (i.e., Wiebe-type functions), wall heat transfer, and work extraction processes. These models are intended to provide only enough detail to compare the global thermodynamics of propagating flame and volumetric (homogeneous) combustion modes. The in-cylinder models can be used separately to study just the combustion by itself or in combination with integrated engine models such as WAVE. We are now using the latter to implement simulations to compare with experimental data from conventional and homogeneous combustion in our Mercedes 1.7-L diesel engine.

As illustrated in Figure 3, our results for idealized combustion processes demonstrate that there is no inherent irreversibility difference between

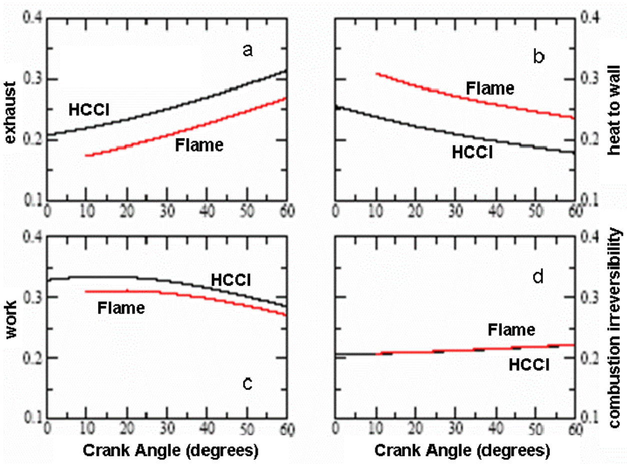

Figure 3. Comparison of ideal HCCI and conventional combustion of stoichiometric hydrogen in air. Vertical axes indicate fraction of original fuel availability distributed to a) exhaust, b) the wall, c) piston work, and d) lost to combustion irreversibility as functions of crank angle in the combustion stroke.

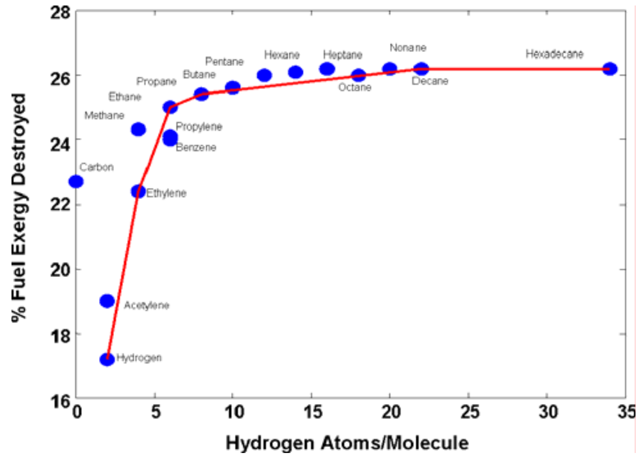

Figure 4. Comparison of combustion irreversibility for adiabatic, constant-volume combustion of different fuels. The initial fuel condition is 298 K, 1 atm.

propagating flame and homogeneous combustion (e.g., HCCI). This is because the same net internal heat transfer is present in both types of combustion. This result is important because it appears to confirm that homogeneous combustion modes are not likely to have much impact *per se* on combustion irreversibility. On the other hand, it does appear that homogeneous combustion modes may be able to achieve reduced wall heat transfer, which could still be of benefit to engine efficiency. Experimental confirmation of the irreversibility and heat transfer characteristics of homogeneous combustion is still needed. We are collaborating with Texas A&M to develop and apply a measurement and analysis protocol that can be used to make such assessments from experimental engine data.

Another combustion concept considered in collaboration with the University of Wisconsin has been the matching of combustion and work extraction rates. This idea stems from the recognition that in current engines, the combustion process typically occurs much faster and before work extraction, causing the internal temperature gradients to be much larger than theoretically necessary. On the other hand, carefully controlled expansion of the piston during the combustion process makes it theoretically possible to maintain a nearly constant combustion temperature. Careful analysis of ideally matched combustion-piston-expansion processes has demonstrated, however, that this does not significantly reduce combustion irreversibility. As with homogenous combustion, internal heat transfer between product and reactant gases still occurs during each increment of reaction, yielding the same global entropy increase. This result implies that the major mechanism by which advanced engine combustion and piston trajectory controls might improve efficiency will be through reduced wall heat transfer, not reduced combustion irreversibility.

One combustion concept for which combustion irreversibility is clearly reduced is the utilization of smaller-molecule fuels. As illustrated in Figure 4, fuels such as hydrogen involve significantly less combustion irreversibility because of the lower entropy generated by disassembling fuel molecules. It appears that the irreversibility trend for most available hydrocarbon fuels correlates well with the fuel hydrogen content. While this reduced combustion irreversibility makes fuels such as hydrogen attractive, one also needs to consider the efficiency (and irreversibility) of the fuel production process in looking at the global energy efficiency picture.

While considering the impact of fuels on combustion irreversibility, we also observed an important constraint that limits the utilization of the increased availability. Specifically, for a single-stage expansion, it is not possible to extract most of the additional energy made available by improving the combustion. Instead, this retained availability is largely passed on to the engine exhaust, and the excess can only be recovered through compound work extraction cycles (e.g., thermo-electrics, bottoming cycles). The effective utilization of hotter exhaust and analysis of compound engine cycles thus appear to offer important opportunities for future study.

High engine compression ratio is another theoretically plausible means for decreasing combustion irreversibility. High compression ratio increases the fuel and air preheating, thus reducing internal heat transfer. In addition, the higher final pressure allows a greater fraction of exhaust gas availability to be extracted as work, reducing the need for cycle compounding. Research and development opportunities associated with higher compression ratios include the development of improved piston sealing systems and materials, high-pressure lubricants, and the measurement and modeling of the impact of such pressures on the combustion kinetics and chemistry.

EGR is used for both emissions control and inducing flameless combustion. In simple terms, EGR involves recycling a fraction of the exhaust gases back into the engine air intake. Currently, these recirculated gases are exposed to large temperature gradients as they mix with the incoming air, further increasing irreversibility. It appears that there may be an opportunity for at least incrementally improving efficiency in the development of advanced heat exchangers that reduce the temperature gradient between these streams. Such development efforts are likely to require consideration of materials of construction, modeling of complex fluid mechanics and heat transfer, and possibly catalytic combustion of unburned hydrocarbons and particulates before or in conjunction with the heat exchange process.

In the longer term, combustion with some type of mediated chemistry will be required to approach the minimum theoretical combustion irreversibility. One example combustion concept proposed in the literature utilizes staged, heterogeneous reactions (reactions on a solid surface) to moderate entropy generation. The basic process involves two reaction steps: 1) a special oxygen storage medium reacts with oxygen from air, and 2) the oxidized storage medium reacts with fuel. One form of this type of combustion (referred to as chemical looping) is being seriously considered for stationary coal combustion. Chemical looping is expected to have applications for large stationary power generation where carbon sequestration is of high priority [4]. For transportation applications, however, much different system designs would be needed in order to avoid solids transport and handling. Specifically, the oxygen storage material would be kept stationary and the air and fuel flows cycled to produce the desired reactions. We refer to this latter type of process as staged combustion with oxygen transfer.

Conclusions

- Our analyses continue to confirm that combustion irreversibility is the single largest contributor to the inefficiency of current engines and that the theoretically possible efficiency of internal combustion engines is >90%.
- Hydrogen and other small-molecule fuels have less combustion irreversibility than conventional fuels such gasoline and diesel, but these advantages may be offset by fuel production penalties.
- Gas-phase homogeneous combustion (such as HCCI) does not appear to be inherently more reversible than conventional combustion, but it may offer incremental efficiency advantages because of reduced wall heat losses.
- Rate-matching between combustion and work extraction in piston engines does not appear to offer any inherent advantages for combustion irreversibility. Some benefits due to less wall heat transfer may be possible.
- Large engine efficiency improvements will only be possible through substantial design changes. Opportunities for near-term incremental efficiency improvements include development of high compression ratio engines, more effective utilization of recirculated exhaust gas heat, and introduction of multiple work extraction stages (i.e., cycle compounding).
- In the longer term, significant reduction of combustion irreversibility will require

modification of the combustion chemistry such that the reactions are more constrained. Staged combustion with oxygen transfer is one approach for implementing such a radically different type of combustion.

FY 2005 Publications/Presentations

1. Presentation at the 9th International Conference on Present and Future Engines for Automobiles in San Antonio, May 29-June 2, 2005, that summarized engine loss mechanisms and recommended research paths.
2. C. S. Daw, K. Chakravarthy, J. C. Conklin and R. L. Graves, "Minimizing Destruction of Thermodynamic Availability in Hydrogen Combustion," International Journal of Hydrogen Energy (In Press, corrected proof available online from 18 August 2005).
3. Stuart Daw, Ron Graves, Kalyana Chakravarthy, Robert Wagner, Scott Sluder, Jim Conklin (ORNL), Dave Foster, Sandy Klein, Ben Druecke (University of Wisconsin), Jerry Caton, Praveen Chavannavar (Texas A&M University), "Seeking More Reversible Combustion for Future Engines (and Implications for HCCI)," Presentation at the HCCI University Working Group Meeting, USCAR, Detroit, September 15, 2005.

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4. Ishida, M. and Jin, H., "A New Advanced Power-Generation System Using Chemical-looping Combustion," *Energy-Int. J.*, *19*, 415, 1994.