II. ADVANCED COMBUSTION AND EMISSION CONTROL RESEARCH FOR HIGH-EFFICIENCY ENGINES

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

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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.

Accomplishments

- Utilized in-cylinder phenomenological models for simulating the efficiency effects of low-temperature combustion modes on thermodynamic availability.
- Continued collaboration with Texas A&M in developing and applying a protocol for analyzing the major exergy losses during engine experiments.
- Continued collaboration with University of Wisconsin and Texas A&M in evaluating the fundamental thermodynamic efficiency limits for conventional engines.
- Participated in National Science Foundation workshop on R&D opportunities for hydrogen combustion.
- In collaboration with Texas A&M and University of Wisconsin presented three papers in the 2006 Technical Meeting of the Central States Section of the Combustion Institute (May 21-23 in Cleveland) summarizing the dominant sources of combustion irreversibility in conventional engines and promising directions for future R&D to increase overall combustion engine fuel efficiency.
- Presented overall results from in-house thermodynamic studies and collaborations with Texas A&M and the University of Wisconsin on stretch engine efficiency to DOE project managers during ORNL site visit in September.
- Identified two novel, unconventional approaches for low-irreversibility combustion suitable for experimental proof-of-principle demonstration.

Future Directions

- Implement and experimentally demonstrate at least one low-irreversibility combustion concept at bench-top scale.
- Continue analyses of data from advanced combustion experiments to determine efficiency implications and appropriate ways to model exergy losses under different operating modes.
- Continue exploring better ways for recuperating exhaust heat and utilizing compound cycles for extracting work.
- 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 (see [1], for example). These studies have demonstrated that both the First and Second Laws of thermodynamics must be taken into accounted in order to understand how efficiently energy is actually utilized. The First Law simply accounts for energy in any form, but the Second Law distinguishes the 'quality' of energy as it relates to producing useful work. For the latter, a thermodynamic property known as availability (or exergy) is tracked as energy is processed by the engine. Because availability directly relates fuel energy to motive work generation, it gives deeper insights into the loss mechanisms for transportation engines than simple energy balances.

In conventional engines the largest efficiency losses (approximately 20-25%) 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 unrestrained chemical 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 existing combustion engines. However, as we discuss below, it is theoretically possible to carry out our 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 1.

In general, combustion irreversibility is mitigated if the reactions take place nearer chemical equilibrium.

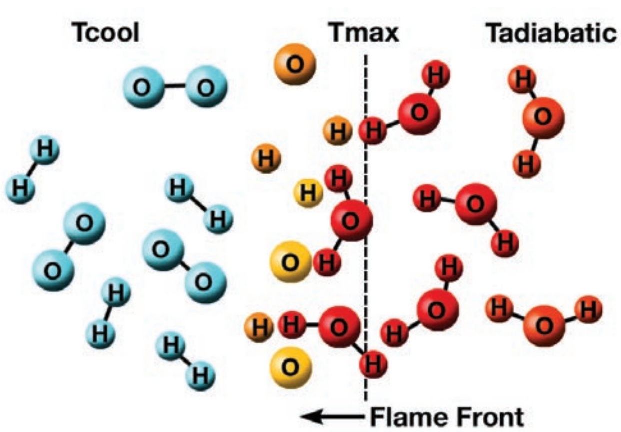

FIGURE 1. Schematic depiction of entropy generation in a flame at the molecular scale. Hydrogen combustion in oxygen is shown for simplicity. Most of the entropy is generated as energetic water molecules share their energy with unreacted oxygen and hydrogen.

This requirement 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 of 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 have been investigating the processes in internal combustion engines (ICEs) that produce availability destruction (i.e., conversion of fuel energy into heat rather than useful work). This year, results from internal modeling studies and collaborations with Prof. Jerry Caton at Texas A&M and Prof. Dave Foster at the University of Wisconsin have been combined to yield a global understanding of the dominant exergy losses in conventional engines, including engines operating in advanced combustion modes. Our thinking has also been significantly impacted by discussions with other pioneers in this area, including John Clarke (Caterpillar, retired), Roy Primus (formerly Cummins, now General Electric), Prof. Noam Lior (University of Pennsylvania), John Farrell and Walt Weissman (Exxon-Mobil), and Prof. Chris Edwards (Stanford University).

The cumulative understanding described above has led to specific recommendations for future R&D activities aimed at improving ICE fuel efficiency, including both experimental and analytical components. Some of these recommended investigations include incremental improvements in existing engines, whereas others involve very novel combustion concepts that go well beyond the constraints of current engines. Our current and future efforts involve a mixture of both types of investigations. As before, we anticipated continued collaborations with those mentioned above, as well as additional collaborations with industrial partners as concepts evolve from theory to experimental practice.

Results

During FY 2006, we have continued utilizing the previously developed computational physical property subroutines for both idealized and experimental engine availability balances. These subroutines have been specifically adapted to simulate and analyze low-temperature combustion modes, which are currently a high priority in DOE fuel efficiency activities. We are now using the latter with experimental data from conventional and homogeneous combustion in the ORNL Mercedes 1.7-L diesel engine. These same routines will be utilized for analysis of results from the ORNL GM 1.9-L engine as it becomes available for experimentation this coming year.

Our updated understanding of the global thermodynamic efficiency limits for conventional engines is based on two types of analyses, one of which considers idealized engine cycles and one of which includes more realistic assumptions about non-ideal engine behavior. As illustrated in Figure 2, our idealized analyses consider global First and Second Law balances around a frictionless conceptual engine that includes a combustion chamber with arbitrarily controlled wall heat losses, isentropic work extraction through a single-stage piston, arbitrarily controlled exhaust gas recirculation (EGR) and/or heat transfer between the exhaust and incoming fuel and air, arbitrary compression ratio, arbitrary air/fuel stoichiometry, and exhaust gas that has fully achieved chemical equilibrium. We consider a large range of fuels (e.g., isooctane, hydrogen, alcohols, etc.) that can burn either homogenously (one zone) or as a propagating flame (two-zone). Burn rates are arbitrarily specified, typically with an adjustable Wiebe function. For more realistic estimates for conventional engines, we add typical non-idealities including mechanical friction, realistic cylinder wall heat transfer, realistic compression ratios, stoichiometric to lean air/fuel mixtures, multi-zone combustion with optimal and non-optimal phasing, and incomplete chemical equilibrium.

An example result coming from the above analyses is illustrated in Figure 3. Here we see a comparison of the net availability changes in an ideal adiabatic engine with stoichiometric, one and two zone combustion of isooctane in air at a fixed global rate. Note that here one-zone combustion is equivalent to the ideal limit for HCCI, while two-zone combustion is equivalent to the ideal limit for propagating flame combustion (e.g., as in a spark-ignited engine). Through such analyses it becomes clear that spatial homogeneity of HCCI does not reduce combustion irreversibility, even though the high spatial gradients of temperature and species surrounding a typical flame are no longer present. This is because the chemical reactions still occur at the same net displacement from equilibrium (as measured in terms of chemical potential), and thus equivalent levels of entropy are generated in the cylinder at the molecular scale. The very slight differences in piston work produced in the two cases here are attributable to slight differences in the

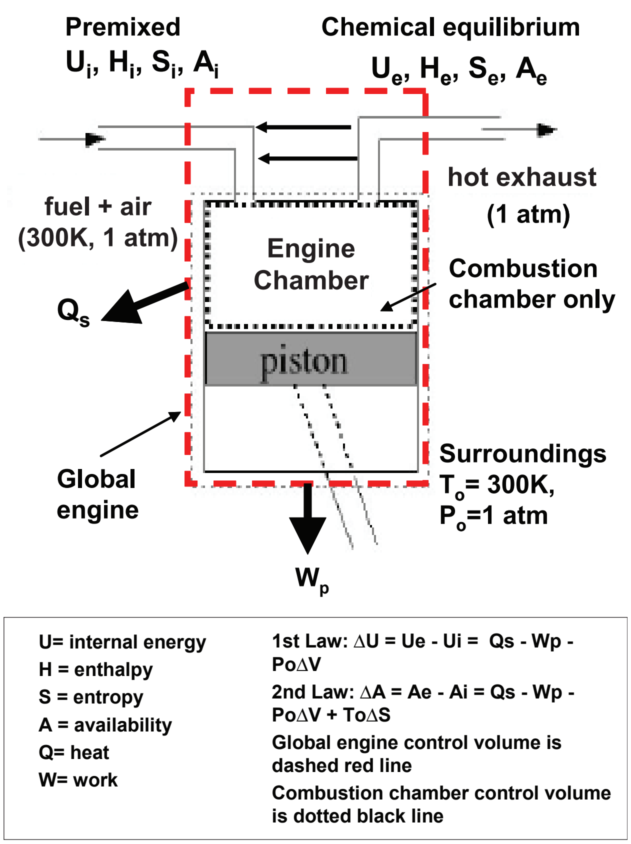

FIGURE 2. Schematic of engine control volumes used for First and Second Law balances. The First Law balances account for overall energy distribution, while the Second Law balances account for thermodynamic availability (which accounts for energy that is converted to entropy and becomes unavailable to do work).

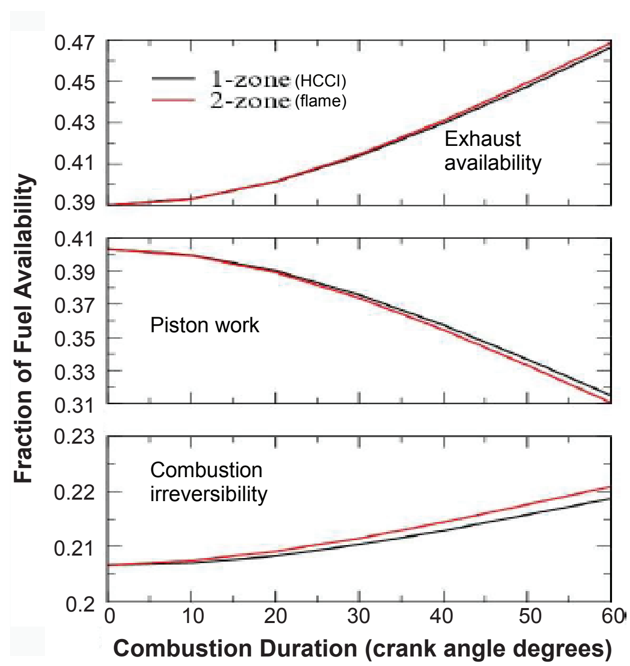

FIGURE 3. Results from an availability analysis of one (HCCI-like) and two-zone (flame-like) combustion simulations for stoichiometric isooctane in air fed to an ideal engine. Here there is no wall heat transfer and burn rate is specified by a Wiebe function. The horizontal axis of each plot is burn duration. The vertical axis is the fraction of the original availability lost on the exhaust, converted to work, and destroyed in combustion, respectively.

effective heat capacity ratios of the gases, which enter into the isentropic work term.

Fuel and air preheating is another parameter expected to reduce combustion irreversibility. Figure 4 illustrates another result from the ideal engine analysis in which the isooctane and air mixture is preheated at constant pressure with recovered exhaust heat before compression in the cylinder. Although combustion irreversibility is reduced as more exhaust heat is recycled, net engine work output is also reduced because more energy is required to achieve the same compression ratio for the expanded inlet charge. The net result of preheating is that the availability lost in the exhaust is increased and overall nothing is really gained. This example illustrates a general trend we have observed repeatedly; reductions in combustion irreversibility in conventional engines are always accompanied by higher losses in the exhaust. This trend points to a fundamental limitation in the ability of single stage engines to extract work from the combustion gases. Ultimately, compound cycles are needed to utilize any additional availability retained by better combustion.

Figures 5 and 6 illustrate how the results of First and Second Law analyses differ from and yet complement each other. In Figure 5, we see the results of a First Law global energy accounting for a non-ideal isooctane-air fueled engine as compression ratio is increased. The output work (at the bottom of the plot) increases with increasing compression ratio, finally becoming almost constant at a compression ratio of about 10. Exhaust energy also decreases with increasing compression ratio, but this decrease is offset by higher heat transfer to the surroundings and more friction. In Figure 6 we see the same type of plot, except that now availability is considered instead of total energy. The exhaust energy now appears in a different light, because it can be seen that only a small portion of this energy is actually available to produce work, especially at higher compression ratios. This implies that attempts to extract this exhaust energy without also reducing availability destruction and/or heat transfer to the surroundings will be less fruitful than one would have otherwise presumed.

As a result of extensive case studies such as those described above, a comprehensive set of conclusions has now been compiled relevant to the fundamental efficiency limits of current engines. Some of the key findings are

- Reduction of combustion irreversibility in single-stage engines will typically cause other losses (e.g., cylinder wall and exhaust heat losses) to increase.
- Cycle compounding is necessary in order to achieve significant benefits from reduced combustion irreversibility.
- Combustion irreversibility is minimized in conventional engines at stoichiometric air/fuel ratios.

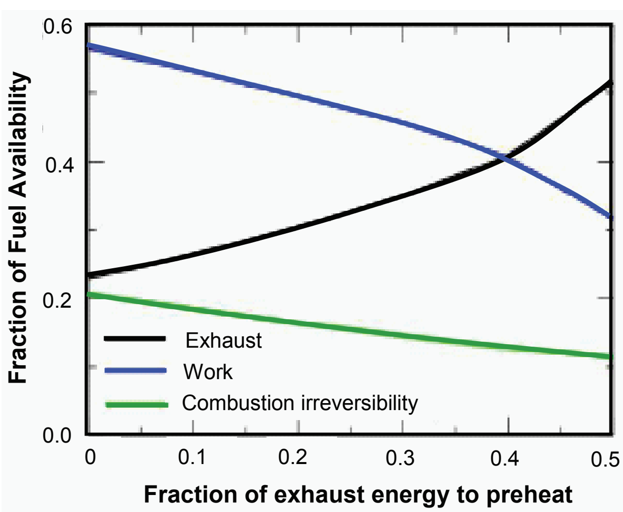

FIGURE 4. Availability results from an ideal engine simulation with recuperative preheating of the isooctane fuel and air. The original fuel availability is accounted for (as fractions) appearing in the exhaust, work, and destruction by combustion irreversibility. The horizontal axis indicates the fraction of the exhaust energy recuperated.

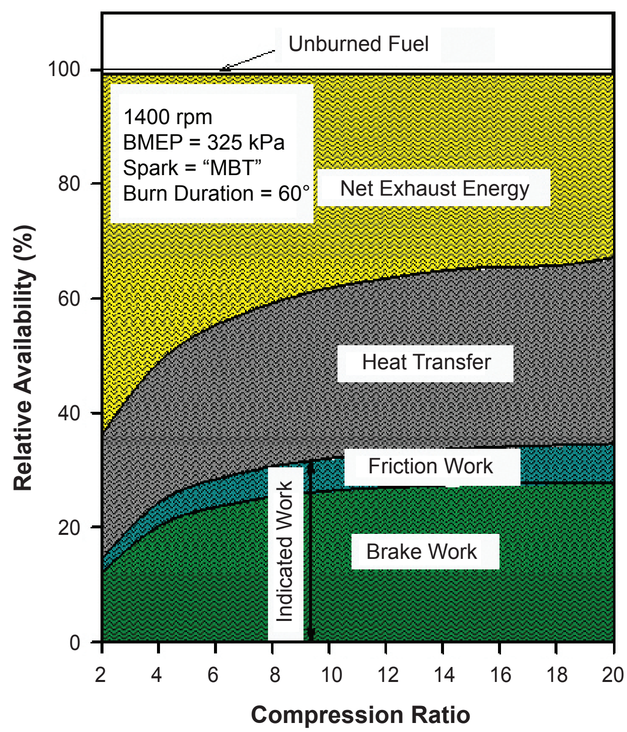

FIGURE 5. Example First Law analysis results for a non-ideal, stoichiometric isooctane-air fuelled spark-ignition engine with varying compression ratio (from Prof. Jerry Caton). As compression ratio increases, work output, friction, and heat transfer all increase.

- Observed benefits in engine work output associated with lean fueling are due to improved gas properties for work extraction (by gas expansion), not because of reduced combustion irreversibility.
- The absence of a flame in HCCI does not reduce combustion irreversibility.
- Observed efficiency advantages associated with HCCI are most likely the result of reduced cylinder wall heat losses.
- Combustion irreversibility is controlled by how far the chemical reactions occur from equilibrium, not how fast the reactions proceed relative the rate of work extraction.

In the longer term, major changes in engine design and mediated combustion chemistry will be required to utilize most of the 20-25% of the fuel energy currently destroyed outright in the combustion process. Radically different combustion approaches such as Staged Combustion with Oxygen Transfer (SCOT) and Counterflow Preheating with near-Equilbirum Reaction (CPER) described in previous reports will probably be required to achieve oxidation reactions that are significantly closer to chemical equilibrium. Shorter-term incremental improvements to existing engines may be possible by judicious use of air and fuel preheating or staging of the combustion reactions (e.g., sequential rich/lean combustion) as long as additional work extraction processes besides the main piston (cycle compounding) are included.

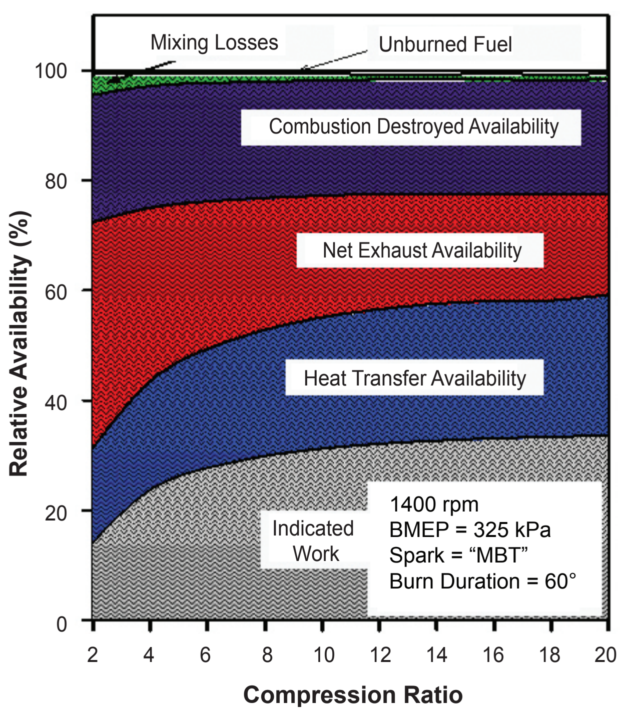

FIGURE 6. Example Second Law analysis results corresponding to Figure 5 (also from Prof. Jerry Caton). Note that much of the energy in the exhaust is actually unavailable to produce work.

Conclusions

Promising engine stretch efficiency concepts which should be considered in the near term include:

- Thermal exhaust heat recuperation combined with compound work extraction;
- Thermo-chemical exhaust heat recuperation with staged gas-phase combustion;
- Low-temperature bottoming cycles for exhaust heat;
- Higher compression ratios;
- Fully expanded engine cycles (e.g., Miller cycles); and
- Exploitation of low-temperature combustion modes with reduced wall heat transfer.

For the longer-term, combustion engines utilizing the following advanced concepts should be considered:

- Heterogeneous combustion reactions (implementations of the SCOT concept);
- Near-equilibrium gas-phase combustion (implementations of the CPER concept);
- Combined cycle systems using both fuel cells and gas-phase reactions;
- High temperature gas-phase combustion with topping cycles (e.g., thermo-photovoltaics); and
- Heterogeneous combustion with mechanical non-gas mechanical work extraction (e.g., piezo-electrics).

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