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, V. K. 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)

Objectives

- Analyze and define specific pathways to improve the thermal efficiency of 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 analyses from the perspective of the Second Law of Thermodynamics as well as the First Law so as to study the large losses inherent in conventional combustion.
- Design and conduct proof-of-principle experiments.

Accomplishments

- Reinforced that the internal combustion engine (ICE) maximum theoretical fuel efficiency approaches 100%, and that a key limiting factor is the high irreversibility in traditional premixed or diffusion flames. These losses, and those from heat transfer during combustion, are the largest losses from a Second Law analysis. The ICE is not a heat engine; hence, direct application of Carnot heat engine principles oversimplifies typical analyses.
- Developed a whitepaper that describes engine loss mechanisms and recommends research paths, and presented it to the FreedomCAR Advanced Combustion and Emission Control Tech Team.
- Initiated modeling and analysis activities at Oak Ridge National Laboratory (ORNL) and the University of Wisconsin to determine whether there are feasible methods to mitigate combustion losses, and to determine whether advanced combustion regimes such as homogeneous charge compression ignition (HCCI) have potential.
- Identified several conceptual pathways to mitigate the losses of thermodynamic availability (exergy) from traditional flames.

Future Directions

- Conduct analysis of data from advanced combustion experiments to determine efficiency implications.
- Develop a protocol to be used in engine experiments that will provide an understanding of where fuel efficiency is being gained/lost when parameters are varied.

- Continue exercising engine and combustion models to identify modifications to the combustion process that would mitigate losses.
- Model and analyze how advanced combustion processes can be best integrated with other engine features for stretching efficiency.

Introduction

Improving engine efficiency is best approached by understanding the losses, then developing ways to mitigate them. Various combinations of analysis and experiments are used in quantifying the thermodynamic losses in engines. A representative distribution of the total available fuel energy to these losses and to useful propulsion (brake) work is shown in Figure 1 [1]. Here we are utilizing a thermodynamic property, availability (or exergy), to study the losses because it gives deeper insight as to the loss mechanisms than a simple energy balance.

The conventional engine combustion process causes the largest losses, which are difficult to mitigate or even explain. These losses are not due to fuel that goes unburned, which is a very small loss. These losses don't even show up on simple "First Law" energy balances for engines. Combustion process losses are associated with the unrestrained chemical reaction of typical combustion processes, and this is where fuel cells gain an advantage over combustion engines. Typical combustion is highly irreversible in the thermodynamic sense and results in destruction of about 20% of the fuel's exergy potential. Most of this irreversibility is associated with so-called 'internal heat transfer' between the products and reactants. Such heat transfer is inevitable in both pre-mixed and diffusion flames,

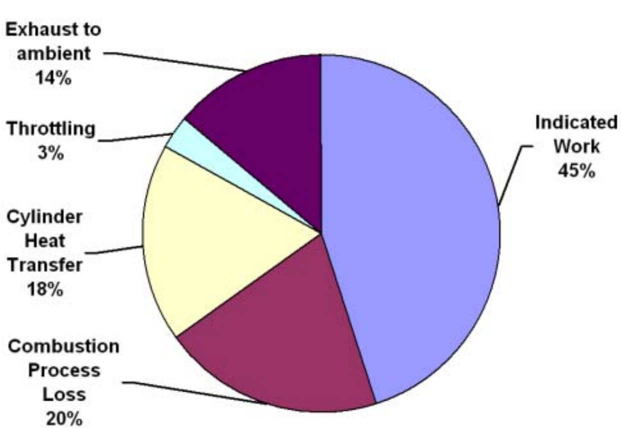

Figure 1. Distribution of Fuel Availability at Full Load, Simulation of Truck Diesel Engine [1]

where highly energetic product molecules are free to exchange energy with unreacted fuel and air molecules [2]. Since these molecules have large energy (i.e., temperature) differences, considerable entropy is generated when they interact. We depict this molecular entropy generation process schematically in Figure 2.

In general, the losses would be mitigated by having the reactions take place nearer equilibrium, bringing reactants to a state closer to the products, reversibly, and by reducing large gradients of temperature or species. These considerations suggest that combustion processes like homogeneous charge compression ignition (HCCI) or low-temperature combustion (LTC) may have some inherent features to reduce combustion reversibility.

Approach

A combination of analyses and experiments will be used to determine the type of engine combustion process that can be devised to reduce the availability destruction in conventional flames. Beginning with an extensive literature review, prior Second Law analyses of engine processes were reviewed for their treatment of this subject. Engine models will be acquired or developed that will perform Second Law calculations and allow introduction of new combustion submodels that address advanced combustion regimes. Commercial codes such as Ricardo WAVE and Gamma Technology GT Power are seen as adequate foundations for this work. Data from various LTC engine experiments at ORNL and elsewhere will be post-processed to determine the exergy losses in the combustion process. Some purposefully designed experiments are likely necessary. Universities will be engaged as appropriate to assist in the development of models and conduct of experiments.

Results

Our literature review of losses associated with typical engine combustion found consistent results that about 20% of the fuel potential is lost in

Table 1. Summary of ICE Efficiency Losses and Pathways to Recover Them

Loss Name	Loss mechanism, description	Potential to improve	Continuous Improvement Path	Breakthrough Path
Combustion process loss	Loss of chemical potential of fuel via unrestrained reaction, dissociation, internal mixing of hot and cool gases.	Large	Higher compression ratio, requiring development in several areas.	"New combustion regimes" dilute combustion with low peak temperatures, high expansion, increased reactant temperature. New thermodynamic strategies and fuel chemistry to lower the temperature of "reversible" combustion. May need variable fuel injection geometries. Methods for very high manifold pressure (boosting). Improved sensors and control methods. Compound compression and expansion cycles.
Exhaust losses	Pressure release and thermal energy.	Large	Miller cycle already has been in commercial use, turbocompounding in limited use in heavy duty diesels.	High expansion ratios achieved by valve timing, turbine expanders, etc. Thermoelectric generators. Lean-NO_x control allowing high compression ratio lean-burn and stratified charge engines. Compound compression and expansion cycles.
Heat transfer loss	Heat transferred to cylinder walls during combustion and expansion.	Large	Improved materials and cooling strategies	Lower temperature combustion, thermal barriers. Downsized engine (low combustion surface area)
Pumping losses	Pressure losses of air and combustion gases. Parasitic engine work to move air and expel combustion products.	Moderate	Improved air management in manifolds and valves.	Fast actuating valves. Improved turbo and air system. Lean-NO_x control to enable unthrottled engines. Variable displacement and compression ratio.
Mechanical friction	Basically rubbing losses.	Moderate	Improved designs for pistons and rings. Rolling contact cam followers in production. Low-friction lubes.	Electromechanical valve system. Lower friction materials and lubes. New component design or engine configuration.
Parasitic losses	Shaft work or fuel consumed to drive auxiliaries and regenerate aftertreatment devices.	Moderate	Electrification of pumps for variable speed and use-on-demand.	New combustion regimes that reduce emissions burden of aftertreatment. Lean-NO_x traps that operate near theorietical requirements of fuel penalty. Combustion regimes that require less fuel pumping

traditional flames. Reference 3 is a good resource for reviewing previous studies. While research and development into other loss mechanisms such as heat transfer and exhaust energy will be very important in improving engine efficiency, progress in reducing combustion irreversibility would be a tremendous and new contribution. A summary of engine losses and technology paths was developed to aid R&D planning for the FreedomCAR Advanced Combustion and Emission Control Tech Team and is shown in Table 1.

Our review also reinforced that the maximum theoretical efficiency of internal combustion engines is oftenunfairly understated by the incorrect application of the Carnot cycle limit. Conventional wisdom holds that internal combustion or reciprocating engines are "heat engines" and are bounded by the maximum theoretical heat engine

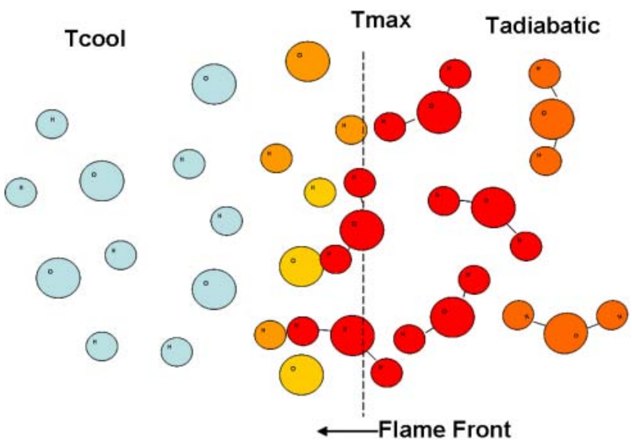

Figure 2. Schematic Depiction of Entropy Generation in a Flame Front (Extremely energetic product molecules dissipate their energy in collisions with surrounding molecules having much lower energy.)

efficiency, known as the Carnot limit. A heat engine, however, has a precise definition: it operates in a thermodynamic cycle, receives heat from a thermal reservoir, produces work from that heat, and rejects heat to a second thermal reservoir. The maximum theoretical efficiency ("Carnot efficiency") of a heat engine is directly related to the temperature difference between the source and sink reservoirs. An internal combustion engine is not a heat engine – there are no thermal reservoirs and the working fluid does not go through a cycle – and thus, its efficiency is not limited to the Carnot cycle efficiency. Moreover, it is widely known that reducing the combustion temperature (as in lean-burn conditions) can increase the engine efficiency, hence departing from the heat engine model. The prevailing notion that all internal combustion engines operate as heat engines in the Otto or Diesel cycle is a simplifying assumption that is useful in education and practical for simple analysis but not theoretically accurate. Both fuel cells and internal combustion engines are subject to the laws of thermodynamics, but neither is bound by the Carnot cycle efficiency. These arguments were articulated in a presentation at the 2004 Diesel Engine Emissions Reduction Conference [4] by Prof. David Foster.

It was recognized, however, that a key tradeoff exists in trying to achieve a more reversible combustion process. Typically, when we configure combustion to occur nearer to equilibrium, we shrink the affinity for reactions to take place and put power density at risk. Paths to mitigate combustion irreversibility were determined to include pre-heating of the reactants (if done reversibly) and better matching of work extraction rate to reaction rate. The latter concept would intuitively approach isothermal combustion.

Analysis of data from a diesel-based LTC experiment at ORNL was started. This engine experiment revealed the interesting situation where peak combustion temperatures were unquestionably lower than conventional due to 90% less NO_x, yet brake thermal efficiency did not decline. This highlights the need for coupling energy and exergy analyses with experiments to track where efficiency is being gained or lost. This will be increasingly important as more emphasis is returned to engine efficiency instead of emission control research, which has been heavily dominant.

The University of Wisconsin was awarded a subcontract to contribute to model development and to study the approach of matching rates of work extraction and combustion reactions. They started with an analysis of availability destruction and Second Law efficiency for constant pressure combustion of hydrogen, methane and octane. In this analysis, the combustion chamber was assumed to be a "black box" in which the properties at the inlet were known and the properties at the outlet were calculated assuming that the fuel-air mixture exited at equilibrium conditions. The purpose of this analysis was twofold. The first reason for this analysis was to compare total availability destruction and Second Law efficiency of octane with the results for hydrogen and methane provided in Dunbar and Lior [2]. The second reason was to provide a precursor to the future study of the distribution of the availability destruction into the underlying mechanisms including heat transfer, chemical reaction and mixing. The analytical results from the University of Wisconsin were very consistent with the earlier work, confirming that the analytical methods are suitable to be exercised further. A notable result is that the exergy destruction per mole of fuel is considerably less for hydrogen than for other fuels. This is consistent with the understanding that exergy destruction is reduced when combustion

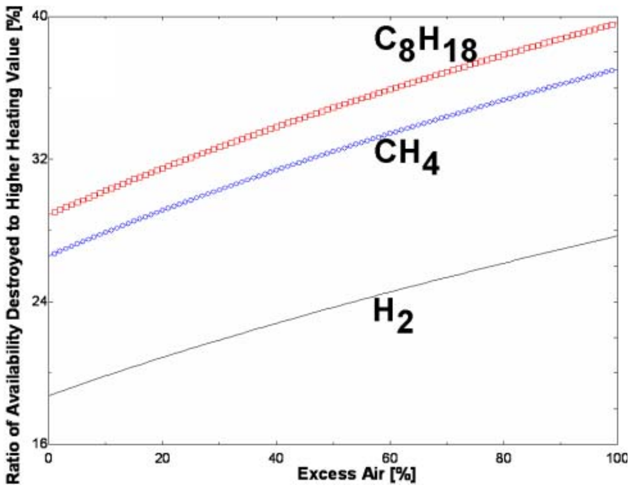

Figure 3. Ratio of Availability Destroyed to Higher Heating Value for Three Fuels at Various Levels of Excess Air

is occurring nearer equilibrium (high temperature) since hydrogen has the highest adiabatic flame temperature of the fuels studied. This is depicted in Figure 3.

Conclusions

- Internal combustion engines have theoretical potential energy conversion efficiency similar to fuel cells (i.e., > 90%).
- The main efficiency losses from current engines are due to combustion irreversibility and heat losses to the surroundings.
- Multiple studies agree that combustion irreversibility losses consume more than 20% of the available fuel energy and are a direct result of flame front combustion.
- The choice of fuel has impact on destruction of availability in combustion, with hydrogen being relatively efficient.
- The potential for volumetric combustion modes, such as HCCI, to reduce combustion irreversibility and wall heat loss has not yet been conclusively determined. Both theoretical and experimental studies focused on Second Law analysis are needed to resolve this issue.

FY 2004 Publications/Presentations

1. Foster, David E., "Are There Practical Approaches for Achieving the Maximum Theoretical Engine Efficiency?," DEER 2004, San Diego, CA, August 2004.
2. Graves, Ron and Murray, Al, "Internal Combustion Engine Efficiency Technology Strategy ('Strawman')," in draft, March 2004.

References

1. Primus, R.J., et al, "An Appraisal of Advanced Engine Concepts Using Second Law Analysis Techniques," Society of Automotive Engineers. SAE 841287, 1984.
2. Dunbar, W.R. and Lior, N., "Sources of Combustion Irreversibility," Combustion Science and Technology, 103, 41-61, 1994.
3. Caton, J.A., "A Review of Investigations Using the Second Law of Thermodynamics to Study Internal-Combustion Engines," Society of Automotive Engineers. SAE 2000-01-1081, 2000.
4. Foster, D.E., "Are There Practical Approaches for Achieving the Maximum Theoretical Engine Efficiency?," DEER 2004, San Diego, CA, August 2004.