Low Exergy Loss Chemical Engines

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Objective: The objective of the proposed research is to enable the development of ultra-high efficiency engines. These engines should convert a much higher fraction of the theoretical exergy limits of their chemical resources to work than the most advanced engines available today.

Background: Improving engine efficiency has long been an objective of engine designers. First-law efficiency (work per unit fuel Lower Heating Value) has improved from less than 1% before 1800 (the Savery and Newcomen engines) to about 70% for compound fuel-cell/gas-turbine engines under development today. However, most simple-cycle engines—best suited for light-duty transportation since the cost, complexity and size issues associated with compounding are avoided—are less than 50% efficient. Spark-ignited (SI, gasoline) engine efficiencies remain in the low to mid 30s, while small-bore direct-injection (DI, diesel) engine efficiencies are in the mid 40s. The generally low simple-cycle efficiencies in current engines can be attributed to significant exergy destruction as well as loss to coolant and environment (i.e., exhaust), all of which can be significantly reduced.

In our previous research for GCEP, we have shown that the engine efficiency problem can best be viewed as one of exergy management. A simple balance equation describing the evolution of resource exergy as a working fluid is transformed by the engine may be written as:

\[ X_{\text{final}} - X_{\text{initial}} = \int dX = \int (\delta X_{\text{in}} - \delta X_{\text{out}} - \delta X_{\text{destroyed}}) \]

Starting with an energy resource (e.g., the fuel) with total exergy \( X_{\text{initial}} \) (thermal and chemical), \( dX \) is a differential change in the amount of exergy contained in the resource, and the \( \delta X \) terms are differential amounts of exergy transferred into or out of the resource, or destroyed by irreversible (i.e., entropy-generating) processes. \( X_{\text{final}} \) is the work-potential (exergy) that remains after the energy resource undergoes a complete engine cycle. High \( X_{\text{final}} \) reflects the overall inability of an engine to extract exergy, thereby leaving it in the resource stream after a complete cycle. The \( \delta X_{\text{out}} \) term consists of both exergy removed from the resource as work and exergy transferred out due to inadvertent losses. The last term \( \delta X_{\text{destroyed}} \) emphasizes that any time entropy is generated, exergy is destroyed and cannot be recovered.

In today’s engines, a large part of the \( \delta X_{\text{destroyed}} \) is a consequence of using an irreversible (unrestrained) approach to chemical energy conversion. This loss is inherent with the use of combustion reactions which by their nature generate entropy. It can only be reduced by re-positioning the reactant state prior to combustion (e.g., compression, which entails investing exergy in the energy resource \( \delta X_{\text{in}} \)) or by switching the engine design away from unrestrained reaction to a restrained form (as is the case with the fuel cell).
**Approach:** The current research addresses the two logical approaches to achieving engine efficiency: minimization of exergy destruction for inherently irreversible (unrestrained) systems and development of new engine designs using reversible (restrained) chemical reaction. In the former case—the branch involving traditional combustion processes—the group will build an experimental apparatus to demonstrate how repositioning the reactant state can drastically reduce exergy destruction in unrestrained reaction. In the latter case, additional theoretical and analytical studies are required in order to understand the thermodynamic design space in a systematic way.

Our previous work has shown that adiabatically compressing the reactants to an extreme pressure is the best way to reduce combustion irreversibility in a simply cycle engine. Entropy generation from the combustion process is minimized when the reactant and product thermodynamic surfaces are closest to one another, as shown in Figure 1.

![Figure 1: Internal energy/entropy/volume thermodynamic surfaces for stoichiometric propane/air. The ideal, reactive Otto cycle is depicted by the black lines while an isentrope with products expanded to the thermal dead state (T0 = 300 K, P0 = 1 atm) is shown in red.](image)

Extreme pressures present the classic problem of high heat transfer rates familiar to all engine designers. We will combat the loss of exergy from the system due to heat transfer by drastically shortening the time that the working fluid spends at the extreme state.

In the experimental portion of the program an ultra-rapid compression/expansion machine will be designed and built in our high-pressure laboratory. We anticipate a final design that includes the capability to conduct a single cycle of the reaction process at a compression ratio of >100:1 and at a rate that is an order of magnitude faster than today’s engines. The apparatus will allow tracking of the piston position so that indicated work can be computed and will have optical access to permit qualitative and quantitative probing of the thermal state and reacting flow conditions within the combustion chamber.

The compression/expansion machine will be used to investigate the extreme compression region of U, V in Figure 1. Various combustion phasing strategies from DI-HCCI through Diesel combustion will be investigated. Performance measurements and calculated quantities such as indicated work, energy lost to heat transfer, and exhaust enthalpy and composition will be
measured over the range of operating conditions. Schlieren-based visualization will be used to observe the spatial structure of the combustion.

The analytical portion of the program will investigate the pathways available to achieving high efficiency through reversible reaction systems. The key development in this work so far is the recognition that electrochemistry is not the only way by which a reversible chemical engine can be constructed. Several hypothetical approaches and engine configurations have been considered, but more work is needed to bridge the hypothetical to that which is demonstrable and to lay the groundwork for new technology options. We will also consider how to systematically organize the design space of compound-cycle engines. As discussed above, if inadequate work extraction capabilities limit the efficiency of simple-cycle machines, use of a compound-cycle strategy can permit significant improvement by converting $\delta X_{out}$ to useful work.

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