

Engine Shows Diesel Efficiency without the Emissions

TRANSPORTATION accounts for 65 percent of U.S. oil consumption. More efficient vehicle engine designs would reduce U.S. dependence on foreign oil and help to mitigate global climate change caused by carbon dioxide emissions. Cleaner engines would contribute to reducing toxic pollutants in the atmosphere, such as nitrogen oxide (NO_x), hydrocarbon (HC), and carbon monoxide (CO). One promising technology is called the homogeneous charge compression ignition (HCCI) engine. Livermore engineers Salvador Aceves and Daniel Flowers are leading a team that is applying modeling processes originally developed by nuclear weapons researchers to study the HCCI engine's potential.

HCCI technology could be scaled to virtually every size and class of transportation engines, from small motorcycles to large ships. Stationary HCCI engines could replace the spark-ignited and diesel engines currently used for backup-power generation and in businesses such as hotels where recovered exhaust heat is used for swimming pools and other facilities. Caterpillar Inc. has donated a six-cylinder stationary engine for the Livermore team to verify modeling results experimentally.

In the HCCI engine, fuel is homogeneously premixed with air, as in a spark-ignited engine, but with a high proportion of air to fuel. When the piston reaches its highest point, this lean fuel-air mixture autoignites (spontaneously combusts) from compression heating, as in a diesel engine. A feature of the HCCI engine is that it burns cooler than spark-ignited and diesel engines. Lower temperature combustion considerably reduces the emissions of nitrogen oxide. In addition, premixed combustion in HCCI engines reduces particulate matter emissions to very low levels. An HCCI engine can operate using any fuel, so long as the fuel can be vaporized and mixed with air before ignition.



Livermore engineers Francisco Espinosa-Loza and Daniel Flowers work on the stationary homogeneous charge compression ignition engine.

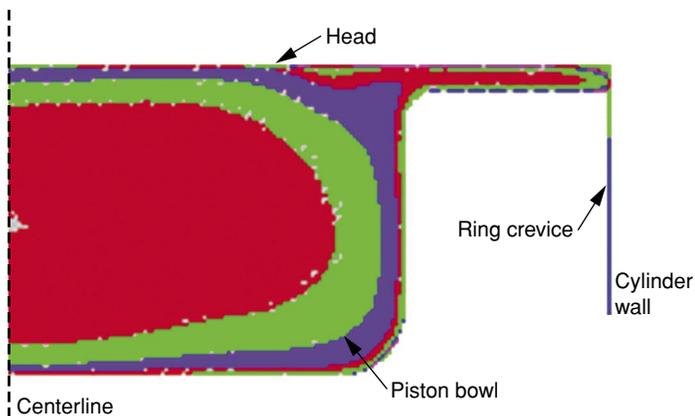
Although the advantages of the HCCI engine are clear, significant challenges must be overcome before the engine is commercially viable. Once engineers resolve these issues, HCCI engines could achieve approximately 40 percent peak efficiency versus 30 percent for spark-ignited engines. Diesel engines can achieve high efficiency similar to HCCI engines, but diesel engines are major sources of NO_x and particulate matter emissions. The Department of Energy's Office of Energy Efficiency and Renewable Energy and the California Energy Commission are funding the Livermore research. Professors Karl Hedrick, Robert Dibble, and J. Y. Chen at the University of California at Berkeley are collaborating with Livermore researchers to address some of the engine combustion control challenges.

Combustion Counts

The greatest challenge is controlling the HCCI engine's ability to operate under a wide range of speeds and loads. The HCCI engine does not have a combustion trigger such as a spark plug or fuel injector found in conventional engines. Instead, combustion is achieved by controlling the temperature, pressure, and composition of the fuel-air mixture so that it spontaneously ignites at the proper time. The required control system is fundamentally more challenging than conventional engines because the ignition is sensitive to very small changes in temperature. When a load is suddenly added, as when a vehicle goes from idle to cruising speed, the control system must adjust the temperature, pressure, and composition rapidly enough to maintain stable combustion.

"Because HCCI engines lack traditional combustion-control systems, understanding the chemical kinetics of combustion is key to addressing its challenges," says Aceves. Livermore's chemical kinetics code, known as HCT, and Los Alamos National Laboratory's fluid mechanics code KIVA, used in combination, have allowed Laboratory researchers to make critical contributions to HCCI technology.

HCT calculates problems involving gas hydrodynamics, transport, and chemical kinetics (how molecules react). The code has been used to study the combustion properties of many compounds. The Livermore team has modified HCT by incorporating models for

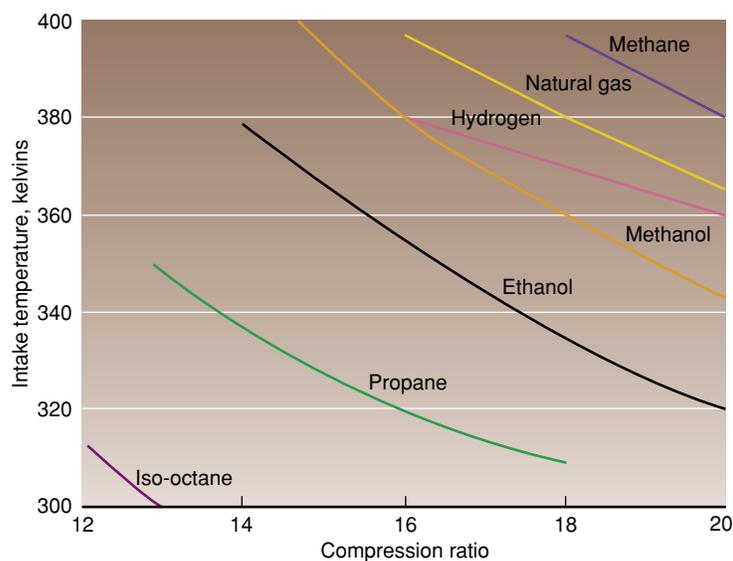


KIVA, a three-dimensional code, is used to simulate gaseous flow in a model of the HCCI engine divided into spatial zones. Together with the HCT code, researchers determine where and when in the combustion chamber the hydrocarbons and carbon monoxide are formed.

heat transfer, a turbocharger, and exhaust-gas recirculation, which are all required for engine analysis.

KIVA is a three-dimensional fluid mechanics code that simulates liquid and gaseous flow under steady-state and transient conditions. Livermore researchers use KIVA to simulate flow in a model of the HCCI cylinder divided into spatial zones. This multizone approach allows temperature and charge velocity distributions to be calculated separately from the much more computationally intensive chemical kinetics processes, which are solved using only a few zones. These codes allow engineers to visualize the inner workings of the combustion process.

Because combustion in HCCI engines is mainly controlled by chemical kinetics and minimally by turbulence effects, the Livermore team developed a two-step process to analyze combustion. The effect of turbulence is first considered by running KIVA to obtain a temperature distribution within the cylinder. The results from KIVA are then used in HCT, which calculates the combustion parameters related to HCCI. This two-step process makes it possible to obtain accurate predictions for the turbulent combustion inside an HCCI engine, within a reasonable computational time for the Laboratory's computers. The significance of this computer-based analysis is that for the first time, researchers can accurately predict combustion rates, emissions, and performance of HCCI engines.



Intake temperatures necessary for various fuels to operate a heavy-duty engine running at maximum power. The intake temperature required for proper ignition is shown as a function of the compression ratio (the ratio of the volume of the combustion space in the cylinder at the bottom of the piston stroke to the volume at the top of the stroke).

Finding the Optimal Fuel

In 2003, Livermore researchers used the HCT and KIVA codes to evaluate fuels and additives that might improve HCCI engine performance. Engineers analyzed several fuels, including propane, methane, natural gas, ethanol, iso-octane, and a variety of additives.

Modeling and experiments have shown that operating conditions for satisfactory HCCI combustion are, in part, dictated by the characteristics of the fuel. Fuels with a relatively low octane number, such as n-heptane or diesel fuel, require lower intake temperatures, and fuels with a high octane number, such as methane and natural gas, require higher intake temperatures. Understanding the limitations of each fuel leads to specific engine design options. Flowers notes, "Certain engine features will work better depending on the type of fuel. We can make any given fuel work with HCCI, but we're still defining the characteristics that work best."

Computer simulations were conducted using small amounts (10 parts per million) of 913 additives to determine if one additive might better control combustion. Some of the peroxides showed the most promise, considerably advancing ignition timing. Although this finding is significant, the benefit of using additives to control combustion must be compared to other potential control mechanisms, such as adjusting the intake temperature to obtain satisfactory ignition timing and combustion. Using an additive may increase the engine's complexity because additional systems would be needed to store and deliver the additive to the combustion chamber.

HCCI's low-temperature combustion also affects its emissions. Although the engine produces lower NO_x and particulate emissions, it releases higher amounts of hydrocarbon and carbon monoxide than spark-ignited or diesel engines. At very low loads, CO levels can reach as high as 60 percent of the total fuel carbon because of incomplete combustion. Fortunately, CO and unburned HC are easily controlled with commercially available oxidation catalysts.

Laboratory researchers used the two-step KIVA-HCT method to investigate when and where in the cylinder the HC and CO are formed. The simulations showed that CO reaches its maximum level immediately following the main heat release during combustion. CO then decreases and slowly rises again during the expansion stroke of the piston. This increase happens because fuel is not completely consumed in the lowest temperature regions of the combustion chamber. Aceves says, "There is enough time during the expansion stroke for unburned fuel to migrate from the crevices and boundary layer into the hot core of the cylinder, where it can react and produce additional CO and CO_2 ."

Because HCCI is a thermal autoignition process, temperature sensitivity is an important issue. Controlling cylinder temperatures will help not only to address the emissions issue but also to control combustion itself. "A few degrees in temperature," says Aceves,

"can make the difference between combustion and no combustion. HCCI needs a control mechanism that detects ambient temperature and adjusts the mixture of air to fuel in the cylinders to obtain ignition at the right time, and the controller has to be fast enough to handle the adjustments." One possibility is for gases coming into the cylinder to be warmed by heat recovered from exhaust gas.

Controlling the temperature is also an important factor for enabling multiple cylinders to work together efficiently. Flowers explains, "Because HCCI is very sensitive to temperature changes, the interactions and differences between cylinders have a greater effect in an HCCI engine than in a spark-ignited or diesel engine."

The Livermore team projects that a stationary HCCI engine will be commercially available in the next five years. Nissan currently sells a hybrid HCCI-diesel automobile in Japan and in Europe. Laboratory engineers are hopeful that in a decade or so, HCCI engines will be powering the transportation industry in the U.S.

—Gabriele Rennie

Key Words: combustion; homogeneous charge compression ignition (HCCI) engine; hydrodynamics, chemistry, and transport (HCT) code; KIVA code.

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