

Homogeneous Charge Compression Ignition (HCCI) Technology

A Report to the U.S. Congress

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HCCI Technology

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Executive Summary

Conference Report 106-914, which accompanied the Department of Interior and Related Agencies Appropriations Act, 2001, P.L. 106-291, requested that the Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) submit a report on Homogeneous Charge Compression Ignition (HCCI) technology. The Conference report also urged the Department of Energy to work with the National Research Council (NRC) to address the potential of HCCI engines. The NRC Standing Committee to Review the Research Program for the Partnership for a New Generation of Vehicles (PNGV) is conducting its seventh review of the PNGV program. On December 7, 2000, the Four-Stroke, Direct-Injection (4SDI) Technical Team briefed the NRC committee on the entire PNGV program. The 4SDI Technical Team included a presentation that summarized the on-going HCCI program and many of the issues discussed in this report. The NRC publication of its examination of the PNGV program is expected in June 2001.

In response to the Congressional request, this report provides a comprehensive overview of the current state-of-the-art in HCCI technology. The report summarizes:

- the benefits of HCCI combustion and the main challenges to the development of commercially viable engines;
- recent developments in HCCI technology and the characteristics of two commercial engines that use HCCI combustion during a portion of their operating range;
- related research currently being performed with support from DOE; and
- potential future directions for HCCI R&D activities.

HCCI combustion has the potential to be highly efficient and to produce low emissions. HCCI engines can have efficiencies as high as compression-ignition, direct-injection (CIDI) engines (an advanced version of the commonly known diesel engine), while producing ultra-low oxides of nitrogen (NO_x) and particulate matter (PM) emissions. HCCI engines can operate on gasoline, diesel fuel, and most alternative fuels. While HCCI has been demonstrated and known for quite some time, only the recent advent of electronic sensors and controls has made HCCI engines a potential practical reality.

HCCI represents the next major step beyond high efficiency CIDI and spark-ignition, direct-injection (SIDI) engines for use in transportation vehicles. In some regards, HCCI engines incorporate the best features of both spark ignition (SI) gasoline engines and CIDI engines. Like an SI engine, the charge is well mixed which minimizes particulate emissions, and like a CIDI engine it is compression ignited and has no throttling losses, which leads to high efficiency. However, unlike either of these conventional engines, combustion occurs simultaneously throughout the cylinder

volume rather than in a flame front. HCCI engines have the potential to be lower cost than CIDI engines because they would likely use a lower pressure fuel-injection system. The emission control systems for HCCI engines have the potential to be less costly and less dependent on scarce precious metals than either SI or CIDI engines. With successful R&D, HCCI engines might be commercialized in light-duty passenger vehicles by 2010, and by 2015 as much as a half-million barrels of primary oil per day may be saved.

HCCI is potentially applicable to both light and heavy-duty engines. Light-duty HCCI engines can run on gasoline and have the potential to match or exceed the efficiency of diesel-fueled CIDI engines, without the major challenge of NO_x and PM emission control or impacting fuel-refining capability. For heavy-duty vehicles, successful development of the diesel-fueled HCCI engine is an important alternative strategy in the event that CIDI engines cannot achieve future NO_x and PM emissions standards.

In fact, HCCI technology could be scaled to virtually every size-class of transportation engines from small motorcycle to large ship engines. HCCI is also applicable to piston engines used outside the transportation sector such as those used for electrical power generation and pipeline pumping. HCCI engines are particularly well suited to series hybrid vehicle applications because the engine can be optimized for operation over a more limited range of speeds and loads compared to primary engines used with conventional vehicles. Use of HCCI engines in series hybrid vehicles could further leverage the benefits of HCCI to create highly fuel-efficient vehicles.

Japan and European countries have aggressive research and development (R&D) programs in HCCI, including both public- and private-sector components. Many of the leading HCCI developments to date have come from these countries. In fact, two engines are already in production in Japan that use HCCI during a portion of their operating range: Nissan is producing a light truck engine that uses intermittent HCCI operation and diesel fuel, and Honda is producing a 2-stroke cycle gasoline engine using HCCI for motorcycles. While HCCI research is on-going in several public and private organizations in the U.S., a real possibility exists that the U.S. lags in the development and implementation of engines using HCCI combustion. For the U.S. automotive and engine industries to maintain their international competitiveness, R&D efforts to develop practical HCCI engines cannot be ignored.

HCCI combustion is achieved by controlling the temperature, pressure, and composition of the fuel and air mixture so that it spontaneously ignites in the engine. This control system is fundamentally more challenging than using a spark plug or fuel injector to determine ignition timing as used in SI and CIDI engines, respectively. The recent advent of electronic engine controls has enabled consideration of HCCI combustion for application to commercial engines. Even so, several technical barriers must be overcome to make HCCI engines applicable to a wide range of vehicles and viable for high volume production. Significant challenges include:

- Controlling Ignition Timing and Burn Rate Over a Range of Engine Speeds and Loads
- Extending the Operating Range of HCCI to High Engine Loads
- Cold-Starts and transient response with HCCI Engines
- Minimizing Hydrocarbon and Carbon Monoxide Emissions

Controlling the operation of an HCCI engine over a wide range of speeds and loads is probably the most difficult hurdle facing HCCI engines. HCCI ignition is determined by the charge mixture composition, its time-temperature history, and to a lesser extent pressure. Several potential control methods have been proposed to control HCCI combustion: varying the amount of exhaust gas recirculation (EGR), using a variable compression ratio (VCR), and using variable valve timing (VVT) to change the effective compression ratio and/or the amount of hot exhaust gases retained in the cylinder. VCR and VVT technologies are particularly attractive because their time response could be made sufficiently fast to handle rapid transients (i.e., accelerations/decelerations). Although these technologies have shown strong potential, performance is not yet fully proven, and cost and reliability issues must be addressed.

Although HCCI engines have been demonstrated to operate well at low to medium loads, difficulties have been encountered at high-load conditions. The combustion process can become very rapid and intense causing unacceptable noise, potential engine damage, and eventually, unacceptable levels of NO_x emissions. Preliminary research indicates the operating range can be extended significantly by partially stratifying the fuel/air/residual charge at high loads (mixture and/or temperature stratification). Several potential mechanisms exist for achieving partial charge stratification, including: in-cylinder fuel injection, water injection, varying the intake and in-cylinder mixing processes, and altering in-cylinder flows to vary heat transfer. The extent to which these techniques can extend the operating range, while preserving HCCI benefits, is currently unknown. Because of the difficulty of high-load operation, most initial concepts involve switching to traditional SI or CIDI combustion for operating conditions where HCCI operation is more difficult. This configuration allows the benefits of HCCI to be realized over a significant portion of the driving cycle but adds the complexity of switching the engine between operating modes.

The fundamental processes of HCCI combustion make cold-starts difficult without some compensating mechanism. Various mechanisms for cold-starting in HCCI mode have been proposed such as using glow plugs, using a different fuel or fuel additive, and increasing the compression ratio using VCR or VVT. Spark-ignition may be the most viable approach to cold-start, though it adds cost and complexity.

HCCI engines have inherently low emissions of NO_x and PM but relatively high emissions of hydrocarbons (HC) and carbon monoxide (CO). Some potential exists to mitigate these emissions at light load by using direct in-cylinder fuel injection. However, regardless of the ability to minimize engine-out HC and CO emissions, controlling HC and CO emissions from HCCI engines will likely require use of an exhaust emission control device. Catalyst technology for HC and CO removal is

well understood and has been standard equipment on gasoline-fueled automobiles for 25 years. In addition, reducing HC and CO emissions from HCCI engines is much easier than reducing NO_x and PM emissions from CIDI engines. However, the cooler exhaust temperatures of HCCI engines may increase catalyst light-off time and decrease average effectiveness. Consequently, achieving stringent future emission standards for HC and CO will likely require some further development of oxidation catalysts for use with HCCI engines.

The U.S. DOE currently has HCCI research activities at two national laboratories and at Stanford University. In addition, DOE included HCCI research aimed at universities as a topic in a solicitation that has recently closed. Although selections and awards have yet to be made, DOE received a number of proposals for HCCI technology R&D. The existing activities are designed to be complementary and consist of the following: 1) an experimental program at Sandia National Laboratories' Combustion Research Facility (SNL/CRF) targeted at understanding the fundamental controlling physics of HCCI with a focus on liquid fuels; 2) a fundamental combustion modeling effort at SNL/CRF; 3) an applied modeling activity at Lawrence Livermore National Laboratory (LLNL) with experimental validation in HCCI engines at the University of California at Berkeley (UCB) focusing on gaseous fuels; and 4) research at Stanford University aimed at investigating the potential of VVT to allow typical SI engines to operate using HCCI under some operating conditions. All four current projects are being conducted in close cooperation with the U.S. automotive and/or heavy engine manufacturers, with the results presented at regularly scheduled working group meetings.

The PNGV has identified HCCI as a high-risk, long-range alternative technology that is deserving of increased R&D efforts. The PNGV has performed an exhaustive literature search of worldwide R&D on HCCI. In addition, Ford, General Motors (GM), and Cummins Engine Company have performed some research on HCCI. Recent research activities have greatly expanded the understanding of HCCI, its controlling mechanisms, and HCCI engine operation strategies. However, substantially more work is required before heavy and light-duty HCCI engines will be ready for production and able to achieve their potential for low emissions and high fuel economy. The main areas still requiring R&D to overcome the challenges identified include:

- Ignition Timing Control: Research is needed to develop control methods for HCCI engines in order to overcome the challenge of maintaining proper ignition timing as load and speed are varied.
- Combustion Rate Control for High-Load Engine Operation: Research is needed to develop methods that slow the heat release rate in HCCI engines at high-load operation to prevent excessive noise or engine damage.
- Engine Cold-Start: R&D is needed to develop an advanced cold-start concept to overcome the challenge of achieving ignition at low temperatures without compromising warm engine performance.

- **Development of Emission Control Systems:** R&D is needed to develop emission control systems and control strategies to overcome the challenge of excessive HC and CO emissions, particularly at low loads.
- **Achieving Satisfactory Engine Transient Operation:** R&D is needed to develop a fast-response control system to overcome the challenge of maintaining proper ignition timing during rapid variations in engine speed and load.
- **Development of Engine Control Strategies and Systems:** Research is needed to develop a methodology for feedback and closed-loop control of the fuel and air systems to keep the combustion optimized over the load speed range in a production vehicle. New sensors may be needed to achieve this level of control.
- **Development of Appropriate Fuel Systems:** Research is necessary to develop a fuel delivery system because it is a key enabling technology to overcome the challenges of maintaining proper ignition timing, smooth heat release rates, and low HC emissions over the operating range.
- **Overcoming Multi-Cylinder Engine Effects:** R&D is needed to develop intake and exhaust manifold designs for multi-cylinder engines to overcome the challenge of maintaining strict uniformity of the inlet and exhaust flows on each cylinder.
- **Developing and Validating Representative Combustion Models:** R&D is needed to develop computational fluid dynamics (CFD) and combustion models for HCCI engines to overcome the challenge of rapidly and inexpensively evaluating engine geometry and combustion system designs.

The DOE believes that university and industry involvement is essential to carrying out future HCCI R&D activities. The Department anticipates this involvement will include industry review of government-funded projects and cost-shared funding of new projects. DOE will reduce its role as the fundamentals of HCCI become clear and as industry nears the point of commercializing this promising technology. In the interim, the funding DOE has requested for HCCI engine research and development will assist in only resolving the highest risk technical issues, and ultimately R&D will accelerate the introduction of HCCI engines and realization of their potential to reduce petroleum use in the transportation sector.

I. INTRODUCTION

Conference Report 106-914, which accompanied the Department of Interior and Related Agencies Appropriations Act, 2001, P.L.106-291, requested that the Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) submit a report on Homogeneous Charge Compression Ignition (HCCI) technology. This report provides a comprehensive overview of the current state-of-the-art in HCCI technology. Section II summarizes the benefits of HCCI and some of the main challenges remaining to the development of commercially viable engines. Section III presents recent developments in HCCI technology and discusses two commercial engines that use HCCI during a portion of their operating range. Section IV describes the related research currently being performed with support from DOE. Section V lists and describes the potential future directions for HCCI R&D activities. Concluding remarks are provided in Section VI.

A. What is HCCI?

HCCI is an alternative piston-engine combustion process that can provide efficiencies as high as compression-ignition, direct-injection (CIDI) engines (an advanced version of the commonly known diesel engine) while, unlike CIDI engines, producing ultra-low oxides of nitrogen (NO_x) and particulate matter (PM) emissions. HCCI engines operate on the principle of having a dilute, premixed charge that reacts and burns volumetrically throughout the cylinder as it is compressed by the piston. In some regards, HCCI incorporates the best features of both spark ignition (SI) and compression ignition (CI), as shown in Figure 1. As in an SI engine, the charge is well mixed, which minimizes particulate emissions, and as in a CIDI engine, the charge is compression ignited

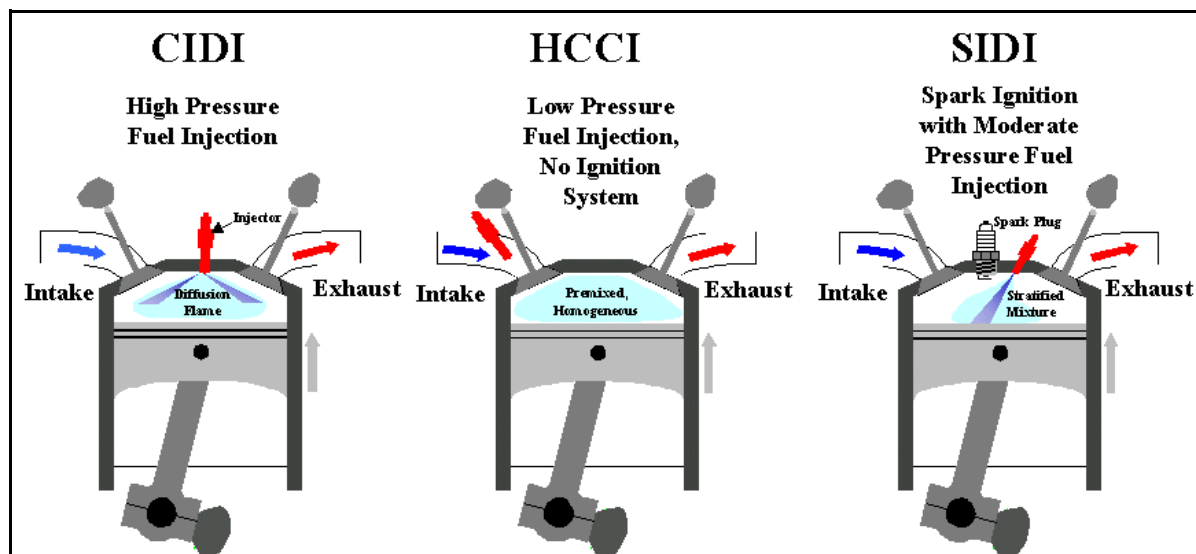


Figure 1. HCCI (as most-typically envisioned) would use low-pressure fuel injection outside the cylinder, and no ignition system. If charge stratification is desired, it may be necessary to use in-cylinder injection.

and has no throttling losses, which leads to high efficiency. However, unlike either of these conventional engines, the combustion occurs simultaneously throughout the volume rather than in a flame front. This important attribute of HCCI allows combustion to occur at much lower temperatures, dramatically reducing engine-out emissions of NO_x .

Most engines employing HCCI to date have dual mode combustion systems in which traditional SI or CI combustion is used for operating conditions where HCCI operation is more difficult. Typically, the engine is cold-started as an SI or CIDI engine, then switched to HCCI mode for idle and low- to mid-load operation to obtain the benefits of HCCI in this regime, which comprises a large portion of typical automotive driving cycles. For high-load operation, the engine would again be switched to SI or CIDI operation. Research efforts are underway to extend the range of HCCI operation, as discussed in the body of this report.

B. What are the Advantages of HCCI?

The advantages of HCCI are numerous and depend on the combustion system to which it is compared. Relative to SI gasoline engines, HCCI engines are more efficient, approaching the efficiency of a CIDI engine. This improved efficiency results from three sources: the elimination of throttling losses, the use of high compression ratios (similar to a CIDI engine), and a shorter combustion duration (since it is not necessary for a flame to propagate across the cylinder). HCCI engines also have lower engine-out NO_x than SI engines. Although three-way catalysts are adequate for removing NO_x from current-technology SI engine exhaust, low NO_x is an important advantage relative to spark-ignition, direct-injection (SIDI) technology, which is being considered for future SI engines.

Relative to CIDI engines, HCCI engines have substantially lower emissions of PM and NO_x . (Emissions of PM and NO_x are the major impediments to CIDI engines meeting future emissions standards and are the focus of extensive current research.) The low emissions of PM and NO_x in HCCI engines are a result of the dilute homogeneous air and fuel mixture in addition to low combustion temperatures. The charge in an HCCI engine may be made dilute by being very lean, by stratification, by using exhaust gas recirculation (EGR), or some combination of these. Because flame propagation is not required, dilution levels can be much higher than the levels tolerated by either SI or CIDI engines. Combustion is induced throughout the charge volume by compression heating due to the piston motion, and it will occur in almost any fuel/air/exhaust-gas mixture once the 800 to 1100 K ignition temperature (depending on the type of fuel) is reached. In contrast, in typical CI engines, minimum flame temperatures are 1900 to 2100 K, high enough to make unacceptable levels of NO_x . Additionally, the combustion duration in HCCI engines is much shorter than in CIDI engines since it is not limited by the rate of fuel/air mixing. This shorter combustion duration gives the HCCI engine an efficiency advantage. Finally, HCCI engines may be lower cost than CIDI engines since they would likely use lower-pressure fuel-injection equipment.

Another advantage of HCCI combustion is its fuel-flexibility. HCCI operation has been shown using a wide range of fuels. Gasoline is particularly well suited for HCCI operation. Highly efficient CIDI engines, on the other hand, cannot run on gasoline due to its low cetane number. With successful R&D, HCCI engines might be commercialized in light-duty passenger vehicles by 2010, and by 2015 as much as a half-million barrels of oil per day may be saved.

Tests have also shown that under optimized conditions HCCI combustion can be very repeatable, resulting in smooth engine operation. The emission control systems for HCCI engines have the potential to be less costly and less dependent on scarce precious metals than either SI or CIDI engines.

HCCI is potentially applicable to both automobile and heavy truck engines. In fact, it could be scaled to virtually every size-class of transportation engines from small motorcycle to large ship engines. HCCI is also applicable to piston engines used outside the transportation sector such as those used for electrical power generation and pipeline pumping.

C. Why is R&D Important for HCCI?

Although stable HCCI operation and its substantial benefits have been demonstrated at selected steady-state conditions, several technical barriers must be overcome before HCCI can be widely applied to production automobile and heavy-truck engines. R&D will be required in several areas, including: controlling ignition timing over a wide range of speeds and loads, limiting the rate of combustion heat release at high-load operation, providing smooth operation through rapid transients, achieving cold-start, and meeting emissions standards. Overcoming these technical challenges to practical HCCI engines requires an improved understanding of the in-cylinder processes, an understanding of how these processes can be favorably altered by various control techniques, and the development and testing of appropriate control mechanisms.

As a result of recent research (see Section III A), the basic principles of HCCI are reasonably well understood. However, in practical engines the air/fuel charge is never completely homogeneous, and creating a charge with an even greater degree of stratification (temperature and/or mixture stratification) appears to have a strong potential for controlling combustion rates to enable high-load operation and for reducing hydrocarbon emissions. (For the remainder of this report, the term HCCI will also be used to refer to variants of HCCI, e.g., partially stratified (i.e., not fully homogeneous) charge compression ignition or SCCI). Research is required to understand how various fuel-injection techniques, methods for introducing EGR, and charge mixing techniques alter HCCI combustion through partial charge stratification. R&D efforts are also needed for the development of fuel-injection hardware and other mixing control techniques that may be required to achieve the desired changes to the in-cylinder processes (e.g., partial stratification). In addition, R&D efforts are needed to investigate control systems such as variable valve timing (VVT) and variable compression ratio (VCR). These controls have a strong potential for controlling HCCI

timing, assisting with cold-start, controlling the engine through transients, and switching into and out of HCCI mode as may be necessary for some applications (see Section III B and Section V). Finally, R&D efforts are needed for the development of sensors and control algorithms for closed-loop control (See Section V F.).

Because of the need to reduce worldwide fuel consumption, greenhouse gas emissions, and criteria air emissions (Federal Tier 2 standards are to be implemented in 2004), there is strong interest in HCCI worldwide. This combustion process stands out as a strong candidate for future automotive and truck engines that consume less fuel while producing substantially lower levels of smog-forming emissions. Japan and several European countries have aggressive R&D programs in HCCI including public and private sector components. Many of the leading developments to date have come from these countries. While HCCI research is ongoing within several public and private organizations in the U.S., there is a real possibility that the U.S. will lag in the development of HCCI, if U.S. research is not expanded. For the U.S. automobile and truck-engine industries to maintain their international competitiveness, R&D efforts are needed to develop practical HCCI engines.

SECTION II. BENEFITS AND CHALLENGES

A. Benefits

A major advantage of HCCI combustion is its fuel-flexibility. Because HCCI engines can be fueled with gasoline, implementation of HCCI engines should not adversely affect fuel availability or infrastructure. (CIDI engines cannot be operated with gasoline due to its low cetane number.) With successful R&D, HCCI engines might be commercialized in light-duty passenger vehicles by 2010, and by 2015 as much as a half-million barrels of primary oil per day may be saved. Additional savings may accrue from reduced refining requirements for fuels for HCCI engines relative to gasoline for conventional SI technology. In addition to gasoline, HCCI operation has been shown for a wide-range of other fuels. Due to this fuel-flexibility, some HCCI applications (e.g., light-duty vehicles) could use gasoline, while other HCCI applications (e.g., heavy-duty trucks) could use diesel fuel.

HCCI also has advantages as a potential low emissions alternative to CIDI engines in light-, medium- and heavy-duty applications. Even with the advent of effective exhaust emission control devices, CIDI engines will be seriously challenged to meet the U. S. Environmental Protection Agency (EPA) 2004 Tier 2 light-duty emission standards or the newly enacted 2007-2010 standards for trucks. This challenge is difficult to overcome because NO_x and particulate matter emission controls often counteract each other. Moreover, CIDI emission control technologies are unproven, expensive, require the injection of fuel or other reductants into the exhaust stream for NO_x reduction, and currently do not last the life of the engine. These emission control systems would also require the use of more expensive ultra-low-sulfur fuels (less than 15 ppm). In addition to emission control devices, expensive fuel injection equipment will be necessary to control emissions (some estimate fuel injection equipment will account for one-third of engine costs). Although the actual cost and fuel-consumption penalties of CIDI emission controls are uncertain, the use of HCCI engines or engines operating in HCCI mode for a significant portion of the driving cycle could significantly reduce the overall cost of operation, thus saving fuel and reducing the economic burden of lowering emissions.

As an alternative high-efficiency engine for light-duty vehicles, HCCI has the potential to be a low emissions alternative to CIDI and SIDI engines. Intensive efforts are underway to develop CIDI and SIDI engines for automotive applications to improve overall vehicle fuel efficiency; however, both CIDI and SIDI engines face several hurdles. As discussed in the preceding paragraph, the emission control devices to reduce NO_x from CIDI engines have several problems. A similar situation exists for SIDI engines because achieving more efficient operation requires them to operate lean. Consequently, NO_x emission control devices similar to those being developed for CIDI engines are required. In addition, the sulfur content of gasoline will be 30 ppm average and 80 ppm maximum as specified by the EPA Tier 2 light-duty vehicle emission standards, a level that

may be too high for the long term durability of lean NO_x emission control systems. It remains to be seen whether SIDI engines will be developed that can meet the Tier 2 emission standards.

While HCCI engines have several inherent benefits as replacements for SI and CIDI engines in vehicles with conventional powertrains, they are particularly well suited for use in internal combustion (IC)-engine/electric series hybrid vehicles. In these hybrids, engines can be optimized for operation over a fairly limited range of speeds and loads, thus eliminating many of the control issues normally associated with HCCI, creating a highly fuel-efficient vehicle. In addition to the on-highway applications discussed above, it should be noted that the benefits of HCCI engines could be realized in most other internal combustion engine applications such as off-road vehicles, marine applications, and stationary power applications. The resulting benefits would be similar to those discussed above.

B. Challenges

HCCI combustion is achieved by controlling the temperature, pressure and composition of the air/fuel mixture so that it autoignites near top dead center (TDC) as it is compressed by the piston. This mode of ignition is fundamentally more challenging than using a direct control mechanism such as a spark plug or fuel injector to dictate ignition timing as in SI and CIDI engines, respectively. While HCCI has been known for some twenty years, it is only with the recent advent of electronic engine controls that HCCI combustion can be considered for application to commercial engines. Even so, several technical barriers must be overcome before HCCI engines will be viable for high-volume production and application to a wide range of vehicles. The following describes the more significant challenges for developing practical HCCI engines for transportation. Greater detail regarding these technical barriers, potential solutions, and the R&D needed to overcome them are provided in Section V. Some of these issues could be mitigated or eliminated if the HCCI engine was used in a series hybrid-electric application, as discussed above.

1. Controlling Ignition Timing over a Range of Speeds and Loads

Expanding the controlled operation of an HCCI engine over a wide range of speeds and loads is probably the most difficult hurdle facing HCCI engines. HCCI ignition is determined by the charge mixture composition and its temperature history (and to a lesser extent, its pressure history). Changing the power output of an HCCI engine requires a change in the fueling rate and, hence, the charge mixture. As a result, the temperature history must be adjusted to maintain proper combustion timing. Similarly, changing the engine speed changes the amount of time for the autoignition chemistry to occur relative to the piston motion. Again, the temperature history of the mixture must be adjusted to compensate. These control issues become particularly challenging during rapid transients.

Several potential control methods have been proposed to provide the compensation required for changes in speed and load. Some of the most promising include varying the amount of hot EGR

introduced into the incoming charge, using a VCR mechanism to alter TDC temperatures, and using VVT to change the effective compression ratio and/or the amount of hot residual retained in the cylinder. VCR and VVT are particularly attractive because their time response could be made sufficiently fast to handle rapid transients. Although these techniques have shown strong potential (see Section III B), they are not yet fully proven, and cost and reliability issues must be addressed.

2. Extending the Operating Range to High Loads

Although HCCI engines have been demonstrated to operate well at low-to-medium loads, difficulties have been encountered at high-loads. Combustion can become very rapid and intense, causing unacceptable noise, potential engine damage, and eventually unacceptable levels of NO_x emissions. Preliminary research indicates the operating range can be extended significantly by partially stratifying the charge (temperature and mixture stratification) at high loads to stretch out the heat-release event. Several potential mechanisms exist for achieving partial charge stratification, including varying in-cylinder fuel injection, injecting water, varying the intake and in-cylinder mixing processes to obtain non-uniform fuel/air/residual mixtures, and altering cylinder flows to vary heat transfer. The extent to which these techniques can extend the operating range is currently unknown, and R&D will be required. Because of the difficulty of high-load operation, most initial concepts involve switching to traditional SI or CI combustion for operating conditions where HCCI operation is more difficult. This dual mode operation provides the benefits of HCCI over a significant portion of the driving cycle but adds to the complexity by switching the engine between operating modes.

3. Cold-Start Capability

At cold start, the compressed-gas temperature in an HCCI engine will be reduced because the charge receives no preheating from the intake manifold and the compressed charge is rapidly cooled by heat transferred to the cold combustion chamber walls. Without some compensating mechanism, the low compressed-charge temperatures could prevent an HCCI engine from firing. Various mechanisms for cold-starting in HCCI mode have been proposed, such as using glow plugs, using a different fuel or fuel additive, and increasing the compression ratio using VCR or VVT. Perhaps the most practical approach would be to start the engine in spark-ignition mode and transition to HCCI mode after warm-up. For engines equipped with VVT, it may be possible to make this warm-up period as short as a few fired cycles, since high levels of hot residual gases could be retained from previous spark-ignited cycles to induce HCCI combustion. Although solutions appear feasible, significant R&D will be required to advance these concepts and prepare them for production engines.

4. Hydrocarbon and Carbon Monoxide Emissions

HCCI engines have inherently low emissions of NO_x and PM, but relatively high emissions of hydrocarbons (HC) and carbon monoxide (CO). Some potential exists to mitigate these emissions at light load by using direct in-cylinder fuel injection to achieve appropriate partial-charge stratification. However, in most cases, controlling HC and CO emissions from HCCI engines will

require exhaust emission control devices. Catalyst technology for HC and CO removal is well understood and has been standard equipment on automobiles for many years. However, the cooler exhaust temperatures of HCCI engines may increase catalyst light-off time and decrease average effectiveness. As a result, meeting future emission standards for HC and CO will likely require further development of oxidation catalysts for low-temperature exhaust streams. However, HC and CO emission control devices are simpler, more durable, and less dependent on scarce, expensive precious metals than are NO_x and PM emission control devices. Thus, simultaneous chemical oxidation of HC and CO (in an HCCI engine) is much easier than simultaneous chemical reduction of NO_x and oxidation of PM (in a CIDI engine). In addition, HC and CO emission control devices are simpler, more durable, and less dependent on scarce, expensive precious metals.

SECTION III. RECENT DEVELOPMENTS IN HCCI

The PNGV has performed an exhaustive literature search of worldwide R&D on HCCI. Table 1 shows a summary of recent developments in HCCI technology. In addition, Ford, General Motors (GM), and Cummins Engine Company have been performing research on HCCI combustion.

Table 1. Summary of Recent HCCI R&D Activities (1998–2000)

Categories	Total Publications	Publications by Region	
Fundamental understanding and benefit demonstration	33	Japan	20
		U.S.	8
		Europe	5
Gasoline HCCI Control	8	Japan	4
		Europe	4
Diesel HCCI Control	3	Japan	3
Alternative Fuel HCCI Control	6	Japan	4
		Europe	2
Load Extension	5	Japan	3
		Europe	2
Catalysts for HC and CO Emissions Control	2	Japan	1
		Europe	1
Mixture Preparation for Diesel	9	Japan	9
Nissan MK	10	Japan	
New ACE	12	Japan	
Lund Institute of Technology	11	Europe	
Keio University	8	Japan	
Lawrence Livermore National Laboratory	5	U.S.	

Ford motor company has an active research program in HCCI combustion. Researchers are using optical diagnostics in single-cylinder engines to explore viable HCCI operating regimes and to investigate methods of combustion control. In addition, chemical kinetic and cycle simulation models are being applied to better understand the fundamentals of the HCCI process and to explore methods of implementing HCCI technology.

GM, at a research level, is evaluating the potential for incorporating HCCI combustion into engine systems. This work includes assessing the strengths and weaknesses of HCCI operation relative to other advanced concepts, assessing how best to integrate HCCI combustion into a viable

powertrain, and the development of appropriate modeling tools. Work is focused on fuels, combustion control, combustion modeling, and mode transitioning between HCCI and traditional SI or CI combustion. GM is also supporting HCCI work at the university level.

Cummins has been researching HCCI for almost 15 years. Industrial engines run in-house using HCCI combustion of natural gas have achieved remarkable emission and efficiency results. However, Cummins has found that it is quite challenging to control the combustion phasing over a real-world operating envelope including variations in ambient conditions, fuel quality variation, speed and load. Because the new diesel emissions targets are beyond the capability of conventional diesel engines, Cummins is investigating all options, including HCCI, as part of their design palette and future engine strategy.

A. Fundamental Understanding

Over the last few years, a consensus has developed as to the nature of HCCI combustion. It is now generally agreed that HCCI combustion is dominated by local chemical-kinetic reaction rates [1]*, with no requirement for flame propagation. This notion has been supported by spectroscopic data indicating that the order of radical formation in HCCI combustion corresponds to self-ignition rather than flame propagation [2,3]. Recent analytical developments also support the view that HCCI combustion is dominated by chemical kinetics, and an analysis method based on this premise has had considerable success in predicting HCCI combustion and emissions [4]. If a truly homogeneous mixture exists at the time of combustion, turbulence has little direct effect on HCCI combustion, but it may have an indirect effect by altering the temperature distribution and the boundary layer thickness within the cylinder. Small temperature differences inside the cylinder have a considerable effect on combustion due to the sensitivity of chemical kinetics to temperature. As a result, heat transfer and mixing are important in forming the condition of the charge prior to ignition. However, they play a secondary role during the HCCI combustion process itself because HCCI combustion is very rapid.

The chemical kinetics modeling of HCCI combustion has concluded that HCCI ignition is controlled by hydrogen peroxide (H_2O_2) decomposition. Hydrogen peroxide decomposes into two OH^\cdot radicals, which are very efficient at attacking the fuel and releasing energy. Hydrogen peroxide decomposition occurs at a temperature range between 1050 and 1100 K. This fundamental chemistry of HCCI autoignition and combustion is identical to the chemistry of knock in spark-ignition engines. With high-octane fuels, little heat is released prior to this main ignition event at 1050-1100 K; however, with low-octane fuels (e.g., diesel fuel) significant heat-producing reactions begin at temperatures of about 800 K [5]. Although the amount of energy liberated is too small to be considered ignition, these low-temperature reactions quickly drive the mixture up to the

* Numbers in brackets refer to references listed at the end of this report.

1050-1100 K temperature necessary for H_2O_2 decomposition and main ignition. It is this effect that causes HCCI to be sensitive to fuel type [5]. Active radicals (i.e., reactive chemical compounds, such as H, OH, HO_2) present in the exhaust gases do not survive the exhaust and intake strokes and play a very minor role in starting HCCI combustion.

Turbulence introduces great complexity to the analysis of stratified charge SI and CIDI engines. The insensitivity of HCCI combustion to turbulence makes it possible to develop a thorough, accurate method of analysis of HCCI combustion. This powerful analytical tool constitutes a great advantage for HCCI engines.

B. Advancements in Speed and Load Control

Combustion control is the biggest challenge to HCCI engines becoming a commercial success. For this reason, several methods have been proposed for achieving HCCI engine control over the wide range of operating conditions required for typical transportation-engine applications. Control technologies reported in the literature have demonstrated some degree of success, but further R&D efforts are required (see Section V). Some of the proposed methods include:

- Variable compression ratio (VCR): HCCI combustion is strongly affected by the compression ratio of the engine. Therefore, a VCR engine has the potential to achieve satisfactory operation in HCCI mode over a wide range of conditions because the compression ratio can be adjusted as the operating conditions change. Conditions change quickly in vehicular applications; consequently, a fast control system that modifies the compression ratio in fractions of a second is necessary. Several options have been studied to obtain VCR engines. One option is to mount a plunger in the cylinder head whose position can be varied to change the compression ratio [6]. The compression ratio could also be varied by using an opposed-piston engine design having variable phase-shifting between the two crankshafts [7]. SAAB has recently announced the development of another method that is based on a hinged, tilting cylinder arrangement [8]. The DOE has sponsored a unique VCR engine design, which is being developed by Envera and tested at Argonne National Laboratory. Similar to the SAAB approach, the Envera approach varies the distance between the cylinder head and the crankshaft. However, unlike the SAAB approach, the VCR mechanism fits inside the crankcase and is expected to provide a faster response and require less energy. The Envera design will be tested this summer with publication of results to follow. While any of these systems or some other mechanism might succeed, only the variable-position plunger system has been demonstrated in an HCCI engine [6]. For these tests, the plunger was controlled by a hydraulic system allowing its position to be varied during engine operation. The data show that the VCR system is capable of controlling HCCI ignition timing to maintain optimal combustion phasing across a very wide range of intake temperatures and fuel types of varying octane number. Although transient operation and variations in speed and load were not reported, the results suggest that a VCR system with sufficiently fast response time is a strong candidate for HCCI engine speed and load control.

VCR would add some cost and complexity to the engine. SAAB has announced plans to go into production with its VCR system on a conventional SI engine [8].

- Variable valve timing (VVT): VVT can be used to change the trapped compression ratio of the engine (i.e., the amount of compression after the gases are trapped by intake-valve closure), and therefore VVT can achieve a similar effect on HCCI combustion as varying the geometric compression ratio of the engine. An engine could be built with a high geometric compression ratio, with lower trapped compression-ratios being obtained by delaying the closing of the intake valve during the compression stroke. Engines with VVT have the added benefit of allowing changes in the temperature and composition of the incoming charge by retaining hot residual gases from the previous cycle in the cylinder. By varying the amount of hot residual, the temperature and mixture of the new charge can be adjusted. Increasing the temperature of the charge in this manner can be used to induce HCCI combustion even with relatively low geometric compression ratios or under cold-engine conditions. In addition, altering the charge composition with partial mixing of the residual could benefit combustion rate control as will be discussed in Section V. VVT could be implemented in an engine with mechanical, magnetic, or hydraulic valve actuators [9]. Recently, researchers at Stanford University, using an electro-hydraulic VVT system, have shown that HCCI combustion can be induced in an engine with a relatively low (10:1) compression ratio [10]. Stanford also showed that the VVT system could be used to control combustion timing and to switch between SI and HCCI operation from one cycle to the next (see in Section IV D). Like VCR, a VVT system would add cost to the engine; however, several manufacturers already have VVT systems in production or are planning to go into production within the next year or two.
- Ignition-enhancing additives: HCCI engine control could be achieved by using two fuels with different octane ratings. The system could be designed to have a main fuel with a high octane number, while the secondary fuel, with a low octane number, is injected as needed to advance combustion. This procedure has recently been studied for a combination of methane and dimethyl ether (DME) [11]. However, this method typically requires carrying and refilling two fuel tanks. Ideally, the amount of the secondary fuel being consumed would be minimal, and the tank could be refueled only at the maintenance intervals. Alternatively, the addition of ozone to the intake has been shown to be an excellent HCCI ignition improver [7], substantially advancing HCCI combustion even at very low concentrations. The system for producing the ozone is inexpensive and has a fast response, but does require electrical power.
- Thermal control: The possibility also exists to control HCCI combustion by controlling the temperature, pressure, and composition of the mixture at the beginning of the compression stroke. In this methodology, thermal energy from exhaust gas recirculation (EGR) and compression work from a supercharger are either recycled or rejected to obtain satisfactory combustion [12]. The main advantage of this method is its simplicity, since it does not require major engine modifications or use of fuel additives. The disadvantage of this method is that it

may be too slow to react to the rapidly changing conditions that typically exist in transportation applications. A full transient response analysis of this type of system has yet to be performed and would depend on the specific system used.

C. Results Using Different Fuels

One of the advantages of HCCI combustion is its intrinsic fuel flexibility. HCCI combustion has little sensitivity to fuel characteristics such as lubricity and laminar flame speed. Fuels with any octane or cetane number can be burned, although the operating conditions must be adjusted to accommodate different fuels, which can impact efficiency, as discussed below. An HCCI engine with VCR or VVT could, in principle, operate on any hydrocarbon or alcohol liquid fuel, as long as the fuel is vaporized and mixed with the air before ignition.

The literature shows that HCCI has been achieved with multiple fuels. The main fuels that have been used are gasoline, diesel fuel, propane, natural gas, and single- and dual-component mixtures of the gasoline and diesel primary reference fuels (iso-octane and n-heptane, respectively). The applicability of these fuels to HCCI engines is discussed below. Other fuels (methanol, ethanol, acetone) have also been tried in experiments, but with inconclusive results.

- **Gasoline:** Gasoline has multiple advantages as an HCCI fuel. Gasoline also has a high octane number (87 to 92 in the U.S. and up to 98 in Europe), which allows the use of reasonably high compression ratios in HCCI engines. Actual compression ratios for gasoline-fueled HCCI engine data vary from 12:1 to 21:1 depending on the fuel octane number, intake air temperature, and the specific engine used (which may affect the amount of hot residual naturally retained). This compression-ratio range allows gasoline-fueled HCCI engines to achieve relatively high thermal efficiencies (in the range of diesel-fueled CIDI engine efficiencies). A potential drawback to higher compression ratios is that the engine design must accommodate the relatively high cylinder pressures that can result, particularly at high engine loads (see discussion in Section V B). Additional advantages of gasoline include easy evaporation, simple mixture preparation, and a ubiquitous refueling infrastructure.
- **Diesel Fuel:** Diesel fuel autoignites rapidly at relatively low temperatures but is difficult to evaporate. To obtain diesel-fuel HCCI combustion, the air-fuel mixture must be heated considerably to evaporate the fuel. The compression ratio of the engine must be very low (8:1 or lower) to obtain satisfactory combustion, which results in a low engine efficiency. Alternatively, the fuel can be injected in-cylinder, but without air preheating, temperatures are not sufficiently high for diesel-fuel vaporization until well up the compression stroke. This strategy often results in incomplete fuel vaporization and poor mixture preparation, which can lead to particulate matter and NO_x emissions. However, one concept for direct injection of diesel fuel, involving late injection (after TDC) with high swirl, has been successful at thoroughly vaporizing and mixing the fuel before ignition at light loads. This mode of operation is used in

the Nissan MK engine, to be discussed in the next sub-section. In addition, diesel fuel has an extensive refueling infrastructure.

- **Propane:** Propane is an excellent fuel for HCCI. High efficiencies can be achieved with propane-fueled HCCI engines because propane has a high octane number (105). Because propane is a gaseous fuel, it can be easily mixed with air. Some infrastructure also exists for propane. Because it can be maintained as a liquid at moderate pressures, the amount of fuel that can be stored onboard a vehicle is comparable to what can be stored for typical liquid fuels.
- **Natural Gas:** Because natural gas has an extremely high octane rating (about 110), natural gas HCCI engines can be operated at very high compression ratios (15:1 to 21:1), resulting in high efficiency. However, similar to gasoline or propane, the engine design must accommodate the relatively high cylinder pressures that can result. Natural gas is widely available throughout the U.S.

D. Early Applications of HCCI Technology

Currently, two commercially available engines run in HCCI mode over part of their duty cycles. In both cases, HCCI operation is limited to light-load conditions, with the engines reverting to conventional combustion systems at high loads, as discussed below.

Nissan "MK" Combustion System

The "Modulated Kinetics" (MK) system, developed by Nissan [13], incorporates in a regular CIDI engine using diesel fuel. At light load, the engine operates with high swirl, high EGR, and retarded injection timing. Under these conditions, the time required to achieve nearly complete mixing is shorter than the time required for fuel autoignition. Therefore, near-homogeneous combustion occurs. At these low loads, the equivalence ratio is low; therefore, the homogeneous combustion results in extremely low NO_x and particulate matter emissions. Retarded fuel injection generally results in low efficiency. However, reduced heat transfer losses mitigate this problem. Consequently, the original efficiency of the CIDI engine is maintained or slightly improved.

The engine runs in MK mode at low load and switches to regular diesel operation at high loads. Current research efforts are directed at extending the range of operation of the engine in MK mode. The plan is to extend the MK region of operation to include the entire area of the load/speed map where the 10-15 mode Japanese emissions test takes place. The 10-15 mode test is considered to be representative of urban driving, and it covers an operating range from idle to slightly less than half of the rated load and speed of the engine.

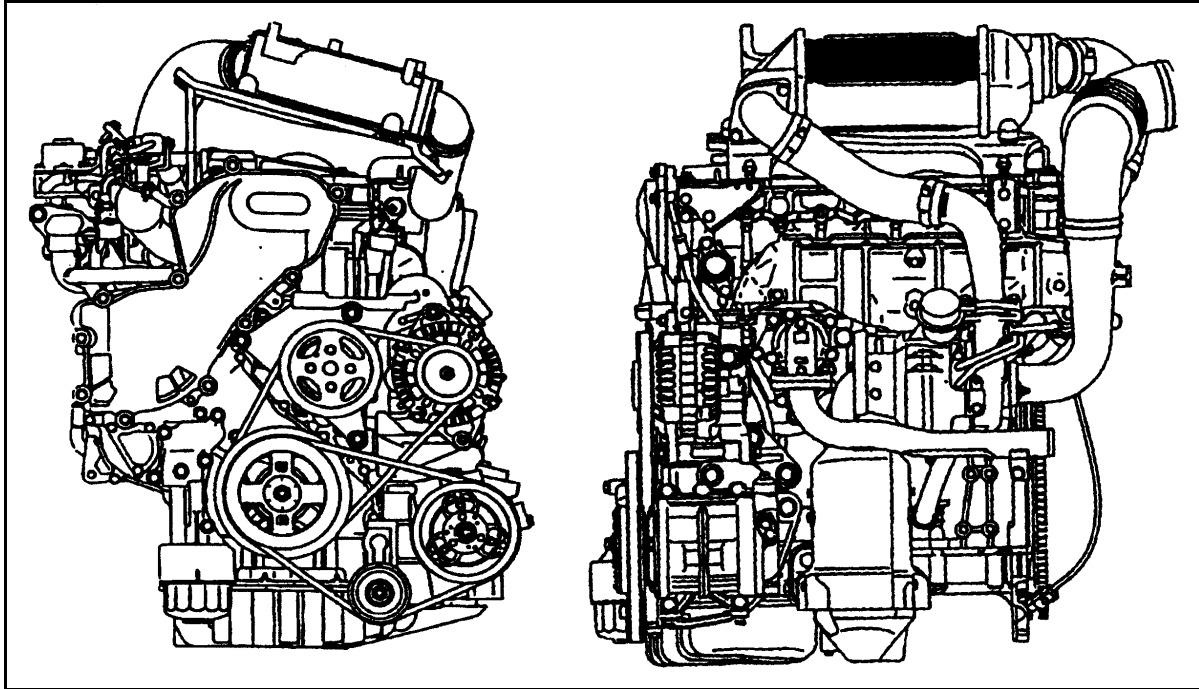


Figure 2. Side and Frontal views of the Nissan MK 2.5 Liter Engine

The MK engine is commercially available in Japan. A 2.5-liter unit went into production in 1998 with a volume of 2000 units per month (see Figure 2). A 3.0 liter engine went into production in 1999 with a volume of 500 units per month, projected to grow to 5000 units per month in the future.

Honda AR Motorcycle Engine

The Honda Active Radical (AR) engine is a 2-stroke cycle, single-cylinder engine that is now commercially available for motorcycles (see Figure 3). The AR engine is also a dual-mode engine. It operates as a spark-ignition engine at high loads, at idle, and for cold-starts. The engine transitions to HCCI combustion at low load. The engine has a low (6.1:1) trapped compression ratio, and HCCI operation is obtained by throttling the exhaust. With exhaust throttling, the engine operates with a high fraction of in-cylinder fuel injection system.)

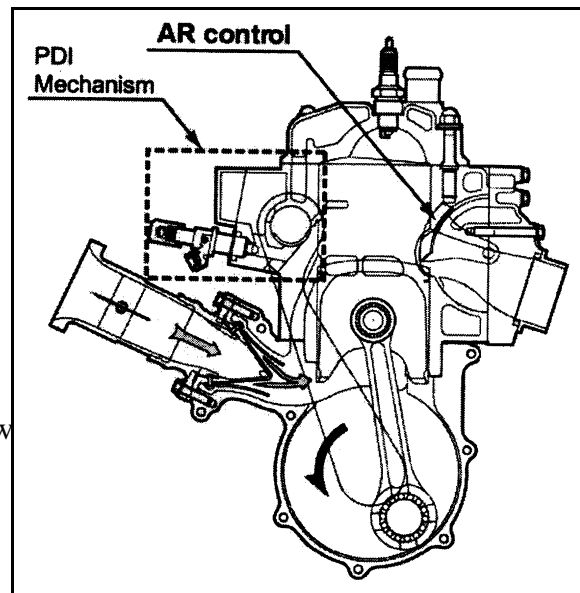


Figure 3. Cut-away of the Honda Active Radical Two-Stroke Cycle Engine (The AR control is a valve that moves to retain residual exhaust gases; the PDI Mechanism is the direct in-cylinder fuel injection system.)

of hot residual gases, which is enough to obtain HCCI combustion, even at a very low compression ratio. Exhaust throttling is decreased as the load increases, until finally the residual fraction is too low to keep the engine operating in HCCI mode. At this point, the engine switches to a conventional spark-ignition operation mode. The performance map has a "transition region" where the engine can operate in both HCCI mode and SI mode.

The AR engine has demonstrated considerable advantages in fuel economy, which is 27 percent better than a regular 2-stroke cycle engine under "real-life" riding conditions [14]. Drivability is also substantially improved. Hydrocarbon emissions are also reduced by 50 percent with respect to a regular 2-stroke cycle engine. However, without emission controls, hydrocarbon emissions are still very high compared to the current automotive emissions standards.

SECTION IV. RELATED RESEARCH BEING PERFORMED WITH FEDERAL SUPPORT

EERE's Office of Transportation Technologies (OTT) is currently supporting HCCI research activities at two national laboratories, a project at Stanford University, and has issued a solicitation for additional university research. OTT has funded HCCI R&D at a total of \$1.5 million over the past two years. The existing activities are designed to be complementary and consist of the following: 1) an experimental program at Sandia National Laboratories' Combustion Research Facility (SNL/CRF) targeted at understanding the fundamental controlling physics of HCCI, with a focus on liquid fuels; 2) a fundamental modeling effort at SNL/CRF focusing on the application of advanced numerical modeling techniques to HCCI combustion; 3) an applied modeling activity at Lawrence Livermore National Laboratory (LLNL) with experimental validation in all-metal engines at University of California at Berkeley (UCB), focusing on gaseous fuels; and 4) research at Stanford University aimed at investigating the potential of variable valve timing (VVT) to extend spark-ignition engines into HCCI combustion regimes under some operating conditions. All four current projects are being conducted in close cooperation with the U.S. automotive and heavy-duty engine manufacturers, with the results presented at regularly scheduled working group meetings. These programs are discussed in detail below, along with a description of the solicitation for new university HCCI research programs.

A. Sandia National Laboratories - HCCI Engine Laboratory

SNL intends to develop the fundamental understanding necessary to overcome HCCI technical barriers (see Sections II and V). To achieve this objective, an HCCI engine laboratory is being equipped with two engines of the same basic design. One, an all-metal engine, will be used to establish operating points, develop combustion-control strategies, and investigate emissions. The other, an optically accessible engine, will be used to apply advanced laser-based and other optical diagnostics to investigate in-cylinder processes, such as mixture preparation using various fuel-injection and residual-mixing techniques, the effects of partial stratification of charge mixture and temperature, the nature of HCCI combustion with various degrees of stratification, and the source(s) of unburned HC emissions. In addition, this project involves a modest computational effort using the CHEMKIN chemical kinetics rate code to investigate trends in HCCI ignition and to provide guidance for engine design and experiments.

1. HCCI Research Engines and Capabilities.

SNL is converting two Cummins B-series CIDI engines into HCCI research engines. This sports utility vehicle-size engine (0.98 liters/ cylinder) was selected because it can provide an operating range relevant to both automotive and heavy-duty manufacturers. The six-cylinder production engines are mounted on either end of a double-ended dynamometer and are being converted for balanced, single-cylinder HCCI operation.

The engines and support facility will provide the flexibility needed to investigate a wide variety of HCCI-like operating modes across a wide load/speed range. This capability is necessary in order to understand the potential of various methods for controlling HCCI ignition, combustion rate, and other HCCI issues, as discussed in Sections II and V. The main features of the laboratory include:

- Compression ratio easily adjustable from 13:1 to 21:1
- Multiple fueling systems (fully-premixed, port injection, and direct injection)
- Flexible fuel capability
- Intake charge tailoring (temperature, pressure, and intake-gas composition)
- EGR/residual-gas mixing
- Variable-swirl capability by customized intake-valve porting
- Optically accessible engine
- Variable valve timing (VVT)

Figure 4 shows a schematic of the laboratory, as it will look after the extended cylinder of the optically accessible engine is completed. Installation of the base-engines, dynamometer, and laboratory sub-systems (e.g., metering and control systems for the intake air and simulated EGR gases, as well as the oil and water circulation and heating systems) is complete. Figure 5 shows a schematic of the optically accessible engine showing a cut away view of the extended cylinder and piston.

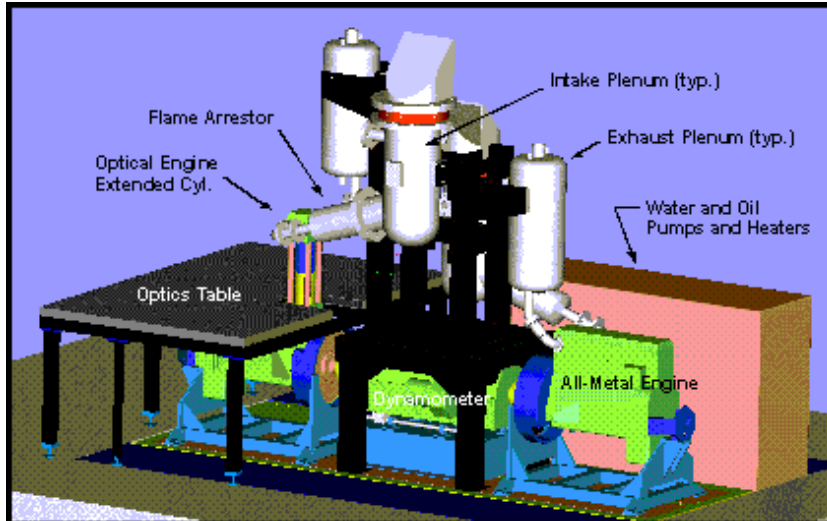


Figure 4. SNL HCCI Laboratory Schematic

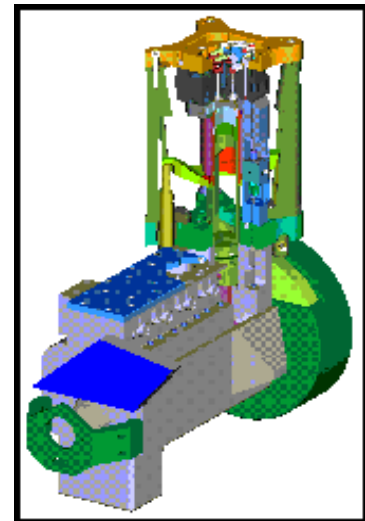


Figure 5. SNL HCCI Optical Engine

2. Chemical-Kinetic Rate Computations

Because the HCCI process is predominantly controlled by chemical-kinetic reaction rates, kinetic-rate computations are being conducted to develop a better understanding of the ignition

behavior of different classes of fuels across the expected operating range. The CHEMKIN code was modified to allow time-varying compression, using the full chemistry mechanisms for n-heptane and iso-octane (from LLNL). These two fuels were selected because their detailed kinetic mechanisms are known and their ignition chemistry spans the range of octane and cetane numbers typical of both diesel fuel and gasoline. This modeling approach, which treats the charge as a single lumped volume, has been shown to provide a good indication of HCCI ignition timing [4], although it is not accurate for predicting combustion rates and peak temperatures. These computations have guided the engine design and will be used to guide future experiments.

Some trends in HCCI ignition timing computed with the CHEMKIN code are presented in Figures 6 and 7 for two surrogate fuels: 1) n-heptane, which has chemistry representative of diesel fuel and 2) iso-octane, which is representative of gasoline. As evident in Figures 6 and 7, ignition chemistry is quite different for these two fuels. For the diesel surrogate (Figure 6), ignition occurs in two stages beginning at a temperature of about 800 K. This ignition temperature limits the compression ratio to 13:1 or less and the efficiency to less than a CIDI engine, in agreement with engine tests in the literature [15]. In contrast, the gasoline surrogate (Figure 7) allows compression to higher temperatures with ignition occurring in a single stage at about 1100 K. This temperature permits higher compression ratios and, therefore, higher efficiencies. Although the compression ratio for the data in Figure 7 is 21:1 (above the optimal range of 15:1 - 18:1), the compression ratios in a real engine will be lower due to inhomogeneities in the charge [6,16], particularly the hot residual from the previous cycle. A lower octane fuel such as 87-octane gasoline could also be used to reduce the compression ratio to the optimal range. HCCI engine tests have shown that using gasoline-like fuels, such as iso-octane, and CIDI-like compression ratios (17:1 - 19:1), HCCI engines can achieve CIDI-like efficiencies and low NO_x emissions [16,17].

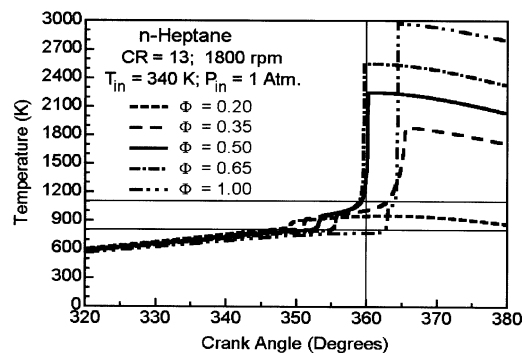


Figure 6. CHEMKIN calculations showing the effect of changes in fuel load on HCCI ignition timing for the diesel-fuel surrogate (n-heptane)

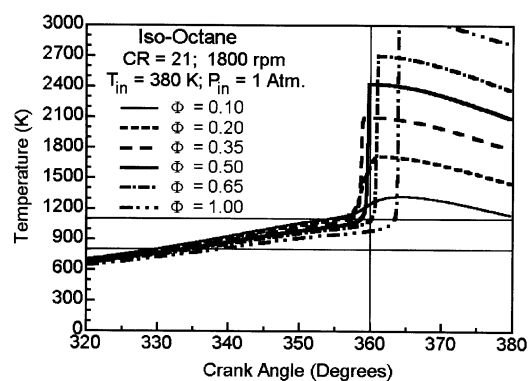


Figure 7. CHEMKIN calculations showing the effect of changes in fuel load on HCCI ignition timing for the gasoline surrogate (iso-octane)

The curves in Figures 6 and 7 show the effect of changing the fuel loading for the diesel and gasoline surrogates. Figure 6 shows that two-stage ignition of a diesel-like fuel results in a wide variation in ignition timing with changes in fuel load; however, with a single-stage ignition fuel, ignition timing varies only a few degrees from low to high load, as shown in Figure 7. Thus, gasoline-like fuels will require less compensation to maintain optimal ignition timing as speed and load are varied over the operating map. A complete discussion may be found in reference [5].

3. Research Directions

Initial research efforts will focus on gasoline-like fuels such as iso-octane, indolene, and gasoline (rather than diesel fuels) for the following reasons: (1) the CHEMKIN code results and other work in the literature show that the ignition characteristics of high-octane, single-stage ignition fuels (e.g., gasoline or natural gas) have significant advantages for HCCI engines compared to fuels like traditional diesel fuel; (2) more volatile liquid fuels like gasoline (or gas-phase fuels) are substantially easier to form into the near-homogeneous mixtures required for HCCI; and (3) liquid fuels have significant advantages in terms of on-vehicle storage, vehicle range, and refueling infrastructure.

Initial experiments will involve establishing baseline HCCI operation using the fully premixed fueling system with iso-octane as the fuel. This operating condition is well defined, easily repeated, and closely matches conditions of the CHEMKIN calculations. After analyzing the ignition timing and combustion rate at the base condition, operating parameters such as intake temperature, engine speed, and fuel load will be systematically varied to establish the operating limits for the fully premixed case. Changes in ignition timing will be compared with CHEMKIN computations to evaluate the predictive capability of this relatively simple model and to determine how the model can be used as a guide in future experiments.

After establishing an understanding of fully premixed HCCI operation, SNL will systematically investigate how changes in mixing, charge preparation, and heat transfer affect HCCI ignition, combustion-rate, and emissions. Many of these studies will focus on understanding and using partial charge stratification as a control mechanism for HCCI and will address technical barriers to implementing HCCI, as discussed in Sections II and V (e.g., controlling ignition timing over the load/speed map, controlling combustion rate at higher loads, and controlling hydrocarbon emissions). Research will include the use of direct-injection fueling to produce partial charge stratification, swirl variation to alter heat transfer rates and in-cylinder mixing, the effects of exhaust/residual gases, and investigations of various mechanisms for exhaust (or residual) gas introduction and mixing to provide controlled partial charge stratification. SNL plans to examine VVT to control HCCI ignition timing over a range of operating conditions and to contribute to partial charge stratification.

With the completion of the optical engine, SNL will investigate the in-cylinder processes using various fueling and mixing schemes. These studies will use advanced laser-imaging diagnostics to

obtain spatially and temporally resolved measurements of the in-cylinder fuel/air/residual mixture. These data will show how the various mixtures affect the nature of HCCI combustion and unburned hydrocarbon emissions. The results of these detailed optical measurements will be correlated with measurements of overall performance from the all-metal engine to provide an understanding of cause-and-effect relationships and to suggest alternative control techniques. The combined results of this project should provide a broad understanding of HCCI and partially stratified, HCCI-like combustion, and will guide HCCI combustion and control strategies.

4. Industrial Interactions

This HCCI engine research project is being conducted in close cooperation with both the automotive and heavy-duty diesel engine industries. SNL consulted industry experts and incorporated their input into the selection of the HCCI research engine, the design of its special features, and the selection of research directions. The results of this project (and some of the fundamental modeling work discussed in the next sub-section) are presented at regularly scheduled cross-cut CIDI cooperative research and development agreement (CRADA) meetings, which include industrial participants from both the CIDI (automotive-sized) CRADA and the Heavy-Duty CIDI CRADA, as well as participants from other research organizations.

Although the HCCI project is not directly a part of either CRADA, it is being conducted in a similar collaborative manner. Presentation of the work at the cross-cut CRADA meeting provides a forum for disseminating the results, having discussions, and getting feedback from representatives of the major U.S. manufacturers of automotive and heavy-duty engines. The industrial partners have reciprocated by presenting results from their HCCI work at these meetings and by providing equipment and expertise for setting up the research engines. Three companies suggested the use of their engines for this project, and the Cummins B-series engine was selected for the reasons discussed above. As part of its participation, Cummins has provided, at no charge, the two engines, spare parts, and technical assistance on converting the engines to single-cylinder operation. Cummins also customized the intake ports of two cylinder heads to provide the required variable-swirl characteristics.

As an outgrowth of industry's strong interest and participation in this project, steps are underway to establish an official memorandum of understanding (MOU) to formalize the partnership between this project and the U.S. engine manufacturers. Under this MOU, the work will continue to be conducted in a collaborative and interactive manner similar to that of the CRADA projects mentioned above.

B. Sandia National Laboratories - Fundamental Modeling

In addition to the HCCI engine experiment, a fundamental study is underway at the SNL/CRF to elucidate the fundamental physics underlying combustion in HCCI engines. This effort is funded by a Laboratory Directed Research and Development (LDRD) award, with support for the

development of the advanced model tools being provided by the DOE Office of Basic Energy Sciences, Chemical Sciences Division (BES/CSD). The study will specifically address a number of challenges faced by HCCI engines such as the control of ignition timing, heat release rate, and emissions over a wide range of loads, speeds, and fuels.

The project will apply advanced modeling tools and is designed to complement work in the HCCI engine laboratory. The specific goals are to: 1) elucidate the role of turbulent mixing in mixture preparation; 2) study the effects of charge inlet conditions, in-cylinder mixing, and engine operating conditions on the ignition delay and heat-release rate; and 3) based on this fundamental knowledge, develop mixture preparation strategies to optimize HCCI combustion over the load-speed map.

1. Advanced Modeling Tools

This study takes advantage of advanced modeling tools developed at the SNL/CRF to incorporate more of the in-cylinder physics than is possible with current codes such as Kiva, CHEMKIN or HCT (Hydrodynamics, Combustion, and Transport). Three new modeling tools will be applied: 1) an extension of one-dimensional turbulence (ODT) modeling to investigate mixing and combustion throughout the engine cycle; 2) a direct numerical simulation (DNS) to examine multi-dimensional mixing effects at small length scales; and 3) large-eddy simulation (LES) to relate the ODT and DNS studies to realistic engine geometries and mixture preparation strategies. Incorporating the detailed physics necessarily increases the computational effort required, and for some models ideal engine geometries will be used. Thus, it is important that these computations be closely associated with the experimental studies at SNL/CRF. Although the added physics will increase computational costs, the knowledge gained will advance the development of more simplistic models and guide hardware development efforts, ultimately leading to substantial savings for the development of HCCI engines.

2. Research Objectives of Fundamental Modeling Research

These advanced modeling techniques for HCCI will optimize strategies for control of ignition timing, heat release rate, and emissions. The models described above will be used for parametric studies over a realistic load-speed map of the joint effects of (1) inlet mixture composition and temperature; (2) in-cylinder mixing strategies including fuel injection and swirl to create partial charge stratification; and (3) engine control through VVT and VCR. The modeling tools take advantage of the detailed chemical kinetics models and can be used to study a variety of fuels. These parametric studies, in conjunction with theoretical analysis, will help evaluate HCCI control strategies that can be tested on the SNL HCCI research engine or on other prototypes. This detailed modeling work should be particularly valuable for investigating the effects of partial charge stratification including:

- C Effects of Charge-Mixture Inhomogeneities: Within practical engines, complete charge homogeneity is unattainable. R&D efforts are being directed at how various mixing strategies

lead to varying inhomogeneities and at how these alter combustion to extend the operating range of HCCI engines. The tools used in this study are uniquely capable of considering the full range of effects arising from inhomogeneities, including their effects on emissions, ignition timing, and heat release rate. Figure 8 shows the temperature history for one representative simulation demonstrating how ODT can be used to model the effects of mixture inhomogeneities and cool walls on HCCI combustion. Even relatively mild inhomogeneities can substantially reduce the heat release rate, as shown by the pressure history curves in Figure 9.

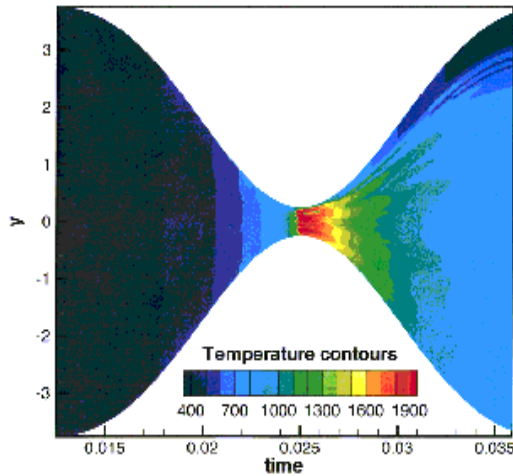


Figure 8. The temperature history in K for a representative ODT simulation. The vertical axis corresponds to a slice through the cylinder. Ignition occurs following compression heating and turbulent mixing.

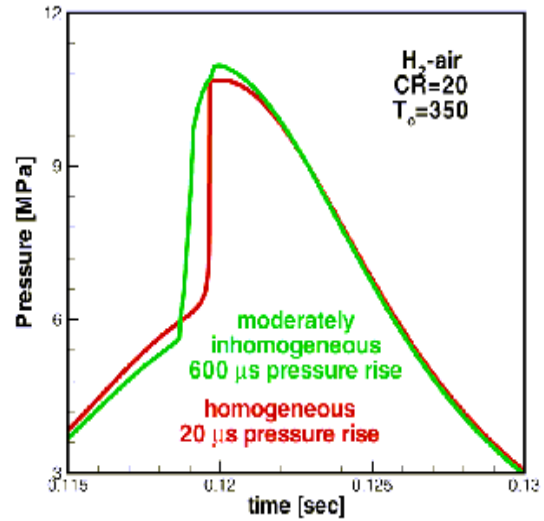


Figure 9. This pressure trace shows the differences between completely homogeneous mixtures and mixtures with small-scale inhomogeneities.

- C Effects of Wall Heat Transfer and the Resulting Thermal Inhomogeneities: These models are also capable of resolving the details of the cool-wall boundary layer and, hence, wall heat-transfer rates. The thermal charge stratification resulting from wall heat transfer is thought to play an important role in controlling heat release rate in addition to HC and CO emissions.

C. Lawrence Livermore National Laboratory (LLNL) - Applied Modeling and Validation

The LLNL activities include detailed modeling of HCCI combustion, studying the fundamentals of HCCI combustion, and finding optimum operating conditions for HCCI engine operation. The experimental work to date includes a single-cylinder engine representative of heavy truck engines and a small, high-speed four-cylinder engine representative of automotive applications. Current research is directed at solving the most important problems associated with HCCI engine operation: speed and load control, cold-start, emissions of HC and CO, power density, and transition to other modes of operation. The LLNL work on HCCI is done in collaboration with UC Berkeley.

1. Analysis of HCCI Combustion

LLNL has developed two powerful HCCI analysis tools: a single-zone model and a multi-zone model. The single-zone model has proven successful in predicting start of combustion and providing reasonable estimates for peak cylinder pressure, indicated efficiency and NO_x emissions, with very little computational cost (5 minutes on an engineering workstation) [18]. The multi-zone model can more accurately predict the combustion process, including HC and CO emissions, at the cost of longer running times (2 hours on an engineering workstation).

The Single-Zone model is being applied to develop detailed engine performance maps and control strategies and to analyze the problem of engine startability. This model shows that an engine operating in HCCI mode is more efficient at low loads at any engine speed than the same engine operating in CIDI mode. The engine has a higher efficiency in HCCI mode due to the faster combustion and the need to delay combustion in order to reduce NO_x emissions in the CIDI engine. The HCCI engine has 72 percent of the maximum torque obtained by the CIDI engine and 88 percent of the power of the CIDI engine, while producing practically zero particulate matter and less than 100 parts per million of NO_x under all operating conditions. Although this simulation has not been validated, it shows the potential of HCCI operation.

The Multi-Zone Model combines a detailed fluid mechanics code with a detailed chemical kinetics code to study fundamentals of HCCI combustion. Figures 10 and 11 display recent results of the multi-zone model. Figure 10 compares experimental and calculated pressure traces for three cases of propane HCCI combustion. Figure 10 shows almost perfect agreement between experimental and numerical pressure traces for Cases 1 and 3. The agreement holds during the compression stroke as well as during the expansion stroke. The multi-zone model has also resulted in excellent predictions for the apparent heat release rates for these cases [19]. Turbulence, flame propagation and mixing make SI and CI combustion much more difficult to accurately predict than HCCI combustion. The model also has the capability of making predictions of HC and CO emissions and to study the effect of cylinder geometry on engine emissions.

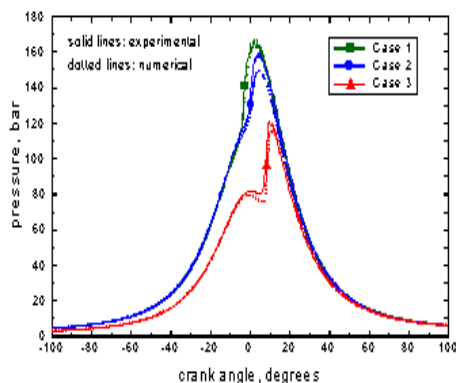


Figure 10. Experimental and numerical pressure traces for three cases of propane HCCI combustion. Dotted lines represent numerical results, and solid lines show experimental results.

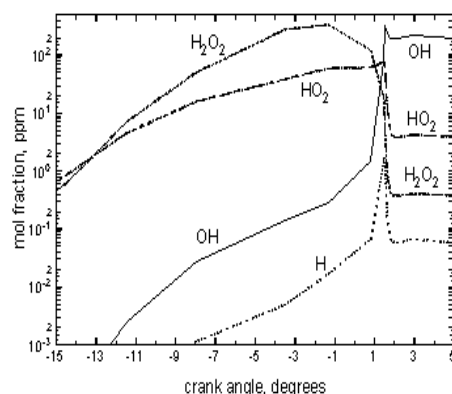


Figure 11. Concentration of H_2O_2 and radicals H, OH, and HO_2 as a function of crank angle [4].

The multi-zone model is also valuable for studying the chemical and physical fundamentals of HCCI combustion. Figure 11 shows the concentration of H_2O_2 and radicals H, OH and HO_2 as a function of crank angle during HCCI combustion. These radicals are selected as the most important for driving the ignition process. In general terms, HCCI ignition occurs when H_2O_2 that has been accumulating in the reactive mixture begins to decompose at a significant rate, producing two hydroxyl (OH) radicals for each H_2O_2 that decomposes. This reaction releases an enormous number of OH radicals, most of which then react with fuel molecules, producing water and heat, increasing the temperature of the reacting mixture, and setting in motion a chain branching sequence. The importance of this reaction is illustrated in Figure 11, where the concentration of H_2O_2 decreases rapidly as OH is being formed.

LLNL has future plans to use the multi-zone model to perform detailed analyses of operating points selected as optimum by the single-zone model. The results will determine an accurate picture of the important operating parameters of HCCI combustion (peak cylinder pressure, indicated efficiency, NO_x , CO and HC emissions). LLNL will use the multi-zone model's results for HC and CO emissions to determine the size and precious metal composition of the catalytic convertor required to meet emissions standards. The detailed model will also be used to study the effect of combustion chamber design on HCCI engine efficiency and emissions. The analysis will evaluate the effect of crevices, piston bowls, swirl, and etc. on engine operation.

2. HCCI Engine Experiments

LLNL will perform engine experiments to validate the application of the models and to implement strategies for HCCI engine startability and control. Current work focuses on a 4-cylinder Volkswagen turbocharged, direct-injection (TDI) compression-ignition engine operating in HCCI mode. (See Figure 12.) This engine has operated in multi-cylinder HCCI mode since October of 1999. (See pressure traces in Figure 13.) TDI engine experiments are used to investigate and validate control strategies for stable HCCI operation over a wide range of speed and load conditions. LLNL will use experiments to investigate control of multi-cylinder interactions and cylinder-to-cylinder variations.

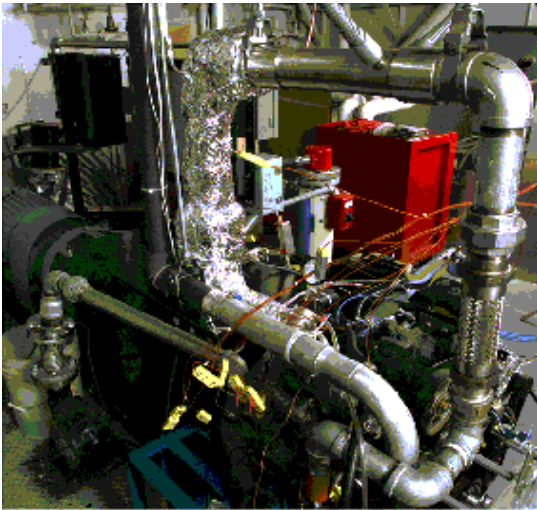


Figure 12. LLNL Experimental HCCI Engine

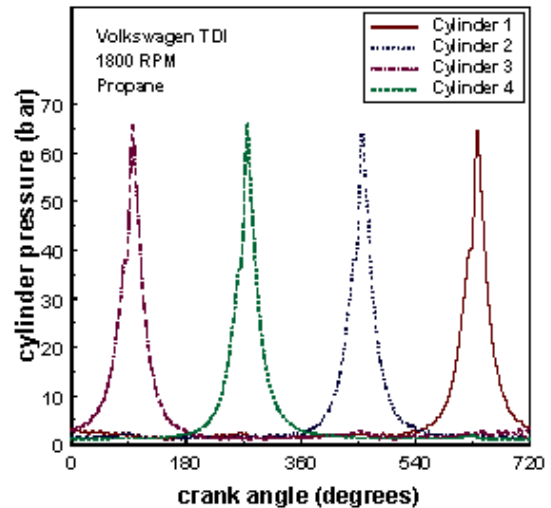


Figure 13. Cylinder Pressure Traces from the LLNL Experimental HCCI Engine

In addition to the TDI engine, LLNL has a Caterpillar 3401 CIDI engine that has been converted to HCCI mode. The Caterpillar 3401 represents a family of engines used in heavy-duty trucks. The converted Caterpillar 3401 engine will run in HCCI mode over a wide range of operating conditions with multiple fuels (e.g., natural gas and propane) to analyze engine performance and to validate the models. This engine will be equipped to handle intake heating, EGR, and fuel additives. LLNL will perform experiments to analyze these control options as well as strategies for starting the engine. Some possibilities include: additives (DME, diesel fuel, etc.), intake preheating, and variable compression ratio.

3. Chemical-Kinetic Model for HCCI Gasoline Combustion

Gasoline consists of hundreds of hydrocarbons, many of which cannot currently be simulated in kinetic models. However, because gasoline is an attractive fuel for HCCI engines, a realistic

chemistry model for gasoline is needed that: (1) can be used in detailed kinetic modeling to predict the beginning and duration of combustion under HCCI conditions and to predict HC, CO, and NO_x emissions; and (2) can serve as a basis for development of reduced chemical kinetic models for inclusion of multidimensional computational fluid dynamic (CFD) models and simplified engineering models of HCCI combustion.

LLNL has found that it is not possible to use familiar fuel parameters such as octane or cetane ratings to guide in the definition of performance ratings of fuels for HCCI combustion. Therefore, a new approach and a new set of ratings for hydrocarbons to identify attractive fuels for HCCI engines are needed.

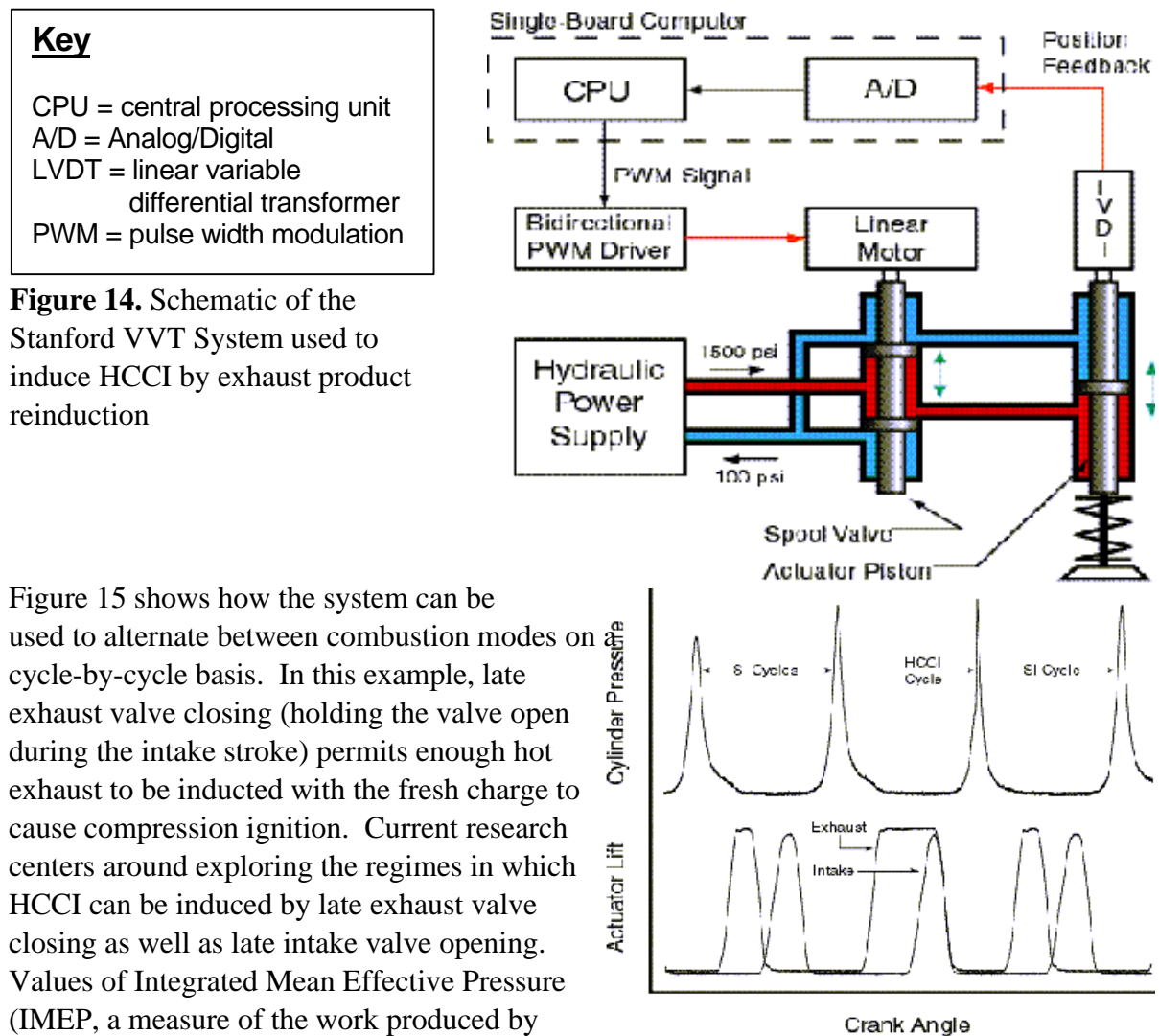
The work required to develop a synthetic (computational surrogate) gasoline suitable for HCCI applications involves computational testing of selected mixtures of hydrocarbons to find one that is able to simulate the performance of gasoline over a wide range of HCCI operating conditions. In addition to fuel classes already quite familiar to modeling efforts, such as large and intermediate size paraffins and olefins, kinetic models for aromatic species such as benzene and toluene, and cycloparaffin species such as cyclopentane and methyl cyclohexane must be developed for inclusion in the surrogate gasoline models. These additional fuel types are important because conventional gasoline contains significant fractions of these types of hydrocarbon species, and their ignition reaction kinetics are quite different from those of other species present in gasoline fuels. This work will use experimental HCCI engine data and require close cooperation between experimental efforts and kinetic modeling experts.

D. Stanford University -- Variable Valve Timing

Stanford University's HCCI studies are focused on how to use Variable Valve Timing (VVT) in order to: 1) induce HCCI over a broad range of operating conditions without the need to throttle and 2) incorporate HCCI into a multi-combustion-mode engine capable of meeting consumer demands for power, PNGV targets for efficiency, and Tier 2 standards for emissions. Both port-fuel injection strategies (minimal cost) and gasoline direct-injection strategies are envisioned, with current emphasis on direct-injection engines. Gasoline is the fuel of choice in this application, and achieving HCCI with low compression ratio and with high-octane fuels is a central aspect of this effort. Key issues that must be addressed include the phasing of the HCCI combustion with piston motion, the dynamic range over which HCCI operation can be achieved, and the development of robust control strategies to manage transitions between optimal combustion regimes as speed/load requirements vary.

Achieving HCCI with low compression ratio (10:1) and with high-octane fuels (propane, octane number = 104) via reinduction (i.e., re-introducing hot combustion products from the previous cycle) has been demonstrated at Stanford. These results were obtained using an electro-hydraulic VVT system developed at Stanford and shown in Figure 14. This system allows arbitrary lift

profiles to be executed by both the intake and exhaust valves. Using this system, a single engine can operate as a conventional, spark-ignition (SI) engine on one operating cycle and execute a completely different mode of combustion on the next cycle. Current capabilities include execution of four of the six major combustion strategies on a cycle-by-cycle basis: homogeneous-charge SI combustion, lean-burn SI combustion, residual-diluted SI combustion, and HCCI. All of these modes can be operated with or without throttling. When throttling is desired, it is provided by the intake valve. All modes can also be operated with advanced breathing strategies including optimal phasing at any engine speed, early- and late-intake-valve closing (Miller cycle), and/or modification of the effective expansion ratio through modification of exhaust valve closing.



discussion of this work may be found in Reference [10].

In the next phase of this work, advanced valve actuation strategies will be employed to expand the operating range of HCCI, and studies aimed at providing optimal phasing of heat release will be conducted. VVT will also be used in conjunction with direct injection in order to demonstrate integration of HCCI into a multimode combustion engine that includes stratified charge and possibly diesel-type fuel injection and combustion. In addition to measurements in conventional (metal) engines, an optically accessible engine tailored for investigating the key parameters of direct injection HCCI with exhaust reinduction is under construction. The data from this experiment will help researchers to develop a quantitative (computational) capability to predict the performance of these new hybrid engines, and it will enable designers to better understand the processes that lead to optimal system performance.

E. Solicitation for HCCI Research

In addition to the currently funded work on HCCI, DOE released a solicitation for proposals for HCCI research by universities and university/industry consortia. Cooperative agreements are expected be put in place at the end of FY2001, based on availability of funding. It is also anticipated that one relatively small cooperative agreement will be let later this year for feasibility demonstration of novel concepts for HCCI by small businesses or universities. The following describes these new initiatives:

1. University Consortium to Conduct HCCI R&D

On November 21, 2000, DOE issued a solicitation for R&D on fuel cells and CIDI engine projects. A small topic was included directed to university research consortia for fundamental HCCI R&D using gasoline. The solicitation was directed to universities due to their strong modeling capability and the high-risk, pre-competitive nature of the R&D. This solicitation recently closed, and the Department received ten proposals addressing HCCI.

The solicitation sought proposals to develop an engine control system that would adjust parameters such as inlet mixture temperature, fuel injection and EGR to allow the HCCI engine to operate over a wider range of speeds and loads than has been demonstrated to date. Enabling technologies such as variable compression ratio, flexible valve timing, variable boost, sensors, and emission control devices may be the basis of proposals as they support HCCI concepts. In addition, proposals were sought to develop control strategies to enable the effective transition from HCCI mode to other potential modes of operation (e.g., direct-injection stratified charge). Proposals were also sought to produce models that will estimate the full-cycle performance and potential fuel economy benefits of the HCCI engine concept.

In addition, proposals were sought to investigate chemical kinetics to model HCCI combustion . Improved modeling of the temperature and pressure histories of the chemical kinetic reacting flow

would greatly assist in development of HCCI combustion systems. Fundamental chemical kinetic mechanism development combined with experimental verification is desired.

The solicitation also requested detailed modeling of the fluid dynamic mixing of the fuel, air and residual products for both Port Fuel Injection (PFI) and Direct Injection (DI) reactant mixing and injection schemes. It is anticipated that complete modeling of the flow for all four strokes (intake, compression, expansion and exhaust) will be necessary to accurately predict the fraction of products left in the cylinder that will be mixed with the fresh charge. Models were sought to provide a detailed understanding of injector behavior, liquid spray atomization, vaporization, and fluid dynamic mixing that is needed for both PFI and DI injection schemes. Models also were sought to compute cycle simulations under various valve timing schemes. To the extent possible, subscale hardware will be used to validate the models and increase understanding of how these technologies fit into a total system design.

These modeling activities will be coordinated with existing DOE programs at national laboratories. The awardee will be asked to establish quantifiable technical targets to measure R&D progress against the technical barriers. The funding to be awarded for this topic will be up to several million dollars (based on available funding) over multiple years. The award will include a 20 percent cost share. An industry technical panel consisting of engine experts will be formed to assist in guiding the university research.

2. CARAT Topic for Homogeneous-Charge Compression-Ignition Enabling Technology

In late 2001, DOE will release a request for new Phase 1 Proposals for its Cooperative Automotive Research for Advanced Technology (CARAT) program. The CARAT program sponsors small businesses and universities to develop advanced, energy-efficient automotive technologies from bench-scale models to engineering-scale prototypes. The CARAT program consists of three phases. In Phase 1, the objective is to prove the feasibility of the technology through building bench-scale models, analyzing performance data, and identifying cost and manufacturing barriers. In Phase 1, DOE typically provides \$150,000 (representing 80% of the total cost); the awardee provides the remaining 20% of the cost-share. Phase 2 focuses on prototype development, and Phase 3 culminates with technology validation. At the end of each phase, DOE selects a few projects to continue to the next phase. Ultimately, DOE matches the developers of these innovative concepts to manufacturers and suppliers for commercialization.

In this solicitation, DOE is including a topic on HCCI R&D to explore hardware feasibility and proof of concept. DOE is seeking proposals (exclusively from small businesses or universities) to develop novel concepts or technologies that will enable the operation of an HCCI engine over a wide range of engine speeds and loads representative of those encountered during light-duty vehicle operation, using gasoline as fuel. DOE seeks to develop hardware for enabling technologies such

as sensors, variable compression ratio, flexible valve timing, variable boost, and emission control devices.

SECTION V. POTENTIAL FUTURE DIRECTIONS FOR RESEARCH AND DEVELOPMENT

As discussed in Section III, recent research has greatly expanded our understanding of HCCI, the controlling mechanisms, and HCCI engine operation strategies. However, substantially more R&D effort is required before heavy and light-duty HCCI engines will be ready for production in the U.S. The main areas requiring R&D are outlined below. In addition, enabling technologies such as VVT are applicable to several of these areas as discussed below.

A. Ignition Timing Control

R&D is needed to develop control methods for HCCI engines in order to overcome the challenge of maintaining ignition timing as load and speed are varied. Maintaining optimal ignition timing is more challenging for HCCI engines than for conventional engines because no positive mechanism, such as spark or fuel-injection, determines ignition timing.

In HCCI engines, ignition timing is determined by the chemical kinetic reaction rates of the mixture, which are controlled by time, temperature, and mixture composition. Of these parameters, ignition timing is most sensitive to temperature. As engine speed and load (time and mixture) are varied, the ignition timing will also vary, unless the charge temperature is adjusted to compensate. Note that the amount of compensation required is a strong function of fuel type, with one-stage-ignition fuels (e.g., gasoline) requiring much less compensation for changes in speed and load than two-stage-ignition fuels (e.g., diesel fuel).

Various methods of controlling the charge temperature near TDC have been suggested and some have been demonstrated for limited conditions. Perhaps the most straightforward way to control charge temperature in an HCCI engine is to add a variable amount of hot EGR to the intake; however, the response is slow, and transients are not handled well. Alternatively, varying the temperature by mechanical variation of the compression ratio (VCR) has recently been demonstrated as an excellent way of controlling HCCI ignition timing [6]. This technique could be adapted to automatic controls. For example, SAAB has recently announced plans to go into production with a variable compression ratio SI engine using a clever tilting-cylinder mechanism, that could easily be adapted to HCCI engines [8]. Finally, VVT might be the most versatile way of controlling the charge temperature. VVT would allow the charge temperature to be varied both by varying the effective compression ratio and by varying the amount of hot residual in the chamber (as demonstrated by the recent work at Stanford University discussed in Section IV D), with the latter having potential advantages for high-load operation and cold-start.

B. Combustion Rate Control for High-Load Operation

R&D is needed to develop methods to slow the rate of combustion in HCCI engines at high engine loads to prevent excessive noise and engine damage. (Due to a combination of relatively slow kinetics and small inhomogeneities in the charge, the heat release rate in HCCI engines is generally slow enough for smooth operation and acceptable noise levels at low and moderate loads. However, at high loads, the kinetic rates are faster, and the heat release rate from near-homogeneous HCCI can become very rapid, causing unacceptable noise and eventual engine damage.) At least two solutions appear feasible as described in the following.

First, on a shorter time horizon, at high loads the engine could switch over and run as a conventional SI or CIDI engine. SI operation has advantages for control of NO_x emissions, and gasoline-like fuels offer additional advantages (as discussed in Section IV). On the other hand, CIDI operation has the advantage of high efficiency. Conversion to SI operation may require reducing the compression ratio, which would be straightforward for an engine equipped with a VVT or VCR system. The recent results from the Stanford VVT engine (Section IV D) indicate that this type of concept can work, but R&D efforts are needed to advance the concept to a wider range of operation and to develop strategies to smoothly transition between HCCI and SI or CIDI operation under load and during strong transients.

Second, the charge temperature and/or mixture could be partially stratified to smooth out the heat release rate. Because even small variations in intake temperature ($\sim 10^\circ \text{C}$) can significantly alter HCCI ignition timing, thermal stratification is a feasible means of spreading out the heat release. Thermal stratification could be accomplished by variable in-cylinder flows that produce non-uniform heat-transfer rates or by incomplete mixing of the cool, fresh fuel/air mixture with hot residual combustion products. In addition to thermal stratification, partial mixture stratification of iso-thermal components (either the fuel/air mixture or the fresh charge/residual mixture) can also produce staged HCCI combustion. The potential of partial charge stratification (thermal and/or species) is largely unexplored. The extent to which stratification can extend the smooth operating range of an HCCI engine is unknown, but it is highly probable that the range could be extended substantially. R&D is required to determine the potential of this technique and to develop practical methods for achieving the required stratification and to investigate whether this stratified operation increases NO_x and particulate matter emissions.

C. Cold-Start

R&D is needed to develop concepts to overcome the challenge of ignition in cold HCCI engines without compromising the warm engine performance. Past research has focused on warm-engine HCCI operation, and little, if any, research has been conducted to address the issue of cold start.

HCCI combustion is strongly dependent on the charge temperature. During cold-start, the fuel/air charge receives no preheating from the intake manifolds and ports, and heat transfer from the compressed charge to the cold combustion chamber walls is high. The combination of these effects can significantly reduce the compressed-gas temperature and prevent an HCCI engine from firing. Three solutions appear possible. First, the engine could be started as a conventional spark-ignition (SI) engine, then switched to HCCI mode after a short warm-up. This scheme would likely require the compression ratio to be reduced during the SI, warm-up operation, which could be readily accomplished on an engine equipped with a VVT or VCR system to handle transients. VVT has the added benefit of allowing the hot residual to be retained from the previous cycle; thereby allowing a more rapid transition to HCCI. (The engine could also be started as a CIDI engine without any compression-ratio adjustment, but gasoline-like fuels offer more advantages, as discussed below.) Second, the engine could be started in HCCI mode by increasing the compression ratio during cold start, with a VVT or VCR system. Third, a glow plug could be used to assist HCCI ignition until the engine warms up. Combinations of these systems might also be used.

D. Emission Control

R&D is needed to develop emission control systems and control strategies to overcome the challenge of maintaining acceptable levels of emissions, particularly at low loads. At low and moderate loads, HCCI engines emit very low levels of NO_x ; consequently, no emissions control is required to reduce NO_x . However, as the operating range is extended to high loads, NO_x emissions can become excessive, and the combustion rate can become too rapid, as discussed previously.

1. Hydrocarbon (HC) and Carbon Monoxide (CO) Emissions: HCCI engines have generally been found to have fairly high HC emissions. At high loads the HC engine-out emissions are similar to those of an SI engine and can probably be controlled with an oxidation catalyst. However, at low loads (e.g., idle) HC emissions become worse, presumably because temperatures are so low that fuel near the wall does not burn. In addition, at very light loads, the temperatures become too low to complete the CO-to- CO_2 reactions. A partially stratified injection scheme would likely mitigate the low-load problems. Rather than having a homogeneous mixture that is very lean throughout, the fuel could be concentrated near the center of the cylinder. Not only would these mixtures burn well in HCCI mode, but fuel would not be near the walls or crevices; therefore, HCs from these sources would also be eliminated. Partially stratified fueling could be accomplished by a DI fuel injection system similar to those being explored for gasoline SIDI engines or by a special intake flow arrangement similar to those used by Mitsubishi and Toyota on their early, stratified charge SI engines. These systems could substantially reduce HCs at low load, but an oxidation catalyst will still likely be required. Research is needed to determine the potential of partial charge stratification techniques or other methods for controlling HC and CO emissions. In addition, R&D efforts are

needed for the development of a low-temperature oxidation catalyst appropriate for HCCI engines operating at light load.

2. NO_x Emissions at High Loads: HCCI engines produce very low levels of NO_x because they operate with a very dilute, premixed charge. As the fuel addition is increased to produce more power, the charge becomes less dilute and combustion temperature increases, which can eventually lead to significant NO_x emissions. For near-homogeneous HCCI engines, the rapid combustion rate at higher loads typically limits the power output before NO_x emissions become excessive. Using partially stratified (in temperature or composition) charge compression ignition (SCCI) as described previously, the operating range could be extended to higher loads but with a more distributed heat release that minimizes peak temperatures and hence NO_x. Research will be required to determine the extent to which fuel load can be increased with SCCI before NO_x emissions become a problem. R&D efforts are required to explore these options and other potentially promising methods to control NO_x at high loads while maintaining the efficiency advantages of HCCI/SCCI-type combustion.

E. Transient Operation

R&D is needed to develop a fast-response control system to overcome the challenge of maintaining proper ignition timing during rapid variations in engine speed and load. Rapid transients present difficulties for current HCCI research engines mainly because the charge temperature is not correctly matched to the operating condition as the speed and load are changing. Transients could be avoided in an electric-hybrid application, which may enable HCCI to enter the marketplace quickly. However, potential HCCI control systems based on devices such as VVT or VCR could be designed with sufficiently fast response to provide smooth, continuous HCCI operation through transients. For example, Stanford University recently demonstrated that a similar VVT system can switch into and out of HCCI combustion from one cycle to the next, as discussed in Section IV D [10]. However, even a less sophisticated VVT system or a VCR system, like the one that SAAB has recently announced, [8] might be adequate. With such a system and good computerized controls, the compression ratio could be varied on a cycle-by-cycle basis to match the exact fueling and speed during a transient. R&D efforts will be required to determine the requisite characteristics of a VVT or VCR system, to develop and test prototype systems, and to develop the necessary control algorithms.

F. Control Systems

R&D is necessary to develop a methodology for feedback and closed-loop control of the fuel and air systems to keep the combustion optimized over the speed and load range of the engine in a production vehicle. Control mechanisms, sensors, and appropriate control algorithms are key enabling technologies for practical HCCI engines. As discussed above, VVT and/or VCR systems have a strong potential for controlling HCCI engines and addressing many of the important issues

such as ignition timing, cold-start, transients, fuel type, and switching into or out of SI mode. Other control mechanisms, such as the use of variable DI fuel-injection timing, various injector types, and various schemes for mixing charge components (fuel, air, and residual combustion products), have strong potential for controlling the rate of heat release, controlling emissions, and allowing the use of different fuel types. In addition, more straightforward methods, such as the introduction of hot EGR into the intake charge, are also applicable.

In addition to the control method and hardware, control algorithms and sensors must be developed to provide feedback for closed-loop control. Under closed-loop control, the engine management system varies engine parameters, such as fuel flow and EGR, in response to inputs from sensors. Closed-loop control allows engine performance and emissions to be continuously optimized during operation. Sensors that might be needed include (but are not limited to) sensors to monitor ignition timing, the rate of combustion heat release, EGR levels, HC emissions, and NO_x emissions. Cost effective sensors durable for engine applications do not currently exist.

Quantification of the potential of many of these control systems for overcoming the technical barriers to HCCI would be conducted as part of the R&D that is outlined in sub-sections A-E above. The control systems used on laboratory HCCI engines would involve custom prototype hardware that is not practical for mass production. In addition to determining the potential of these various methods of HCCI control, R&D efforts are needed to develop practical, economical systems for production HCCI engines. These R&D efforts would include developing economically feasible sensors and control algorithms.

G. Fuel System Development

R&D is necessary to develop a fuel delivery system because it is a key enabling technology to overcome the challenge of maintaining proper ignition timing, smooth combustion rates, and low emissions over the operating range of the engine. Various types of fuel systems have been proposed including port fuel injectors, DI fuel injectors similar to those designed for SI engines, DI diesel engine injectors, and combinations of these injectors. Each type has advantages for different operating regimes and fuel types.

For diesel fuel, the type of injector required depends on the strategy selected for fuel-air mixing and combustion. The most promising approach appears to be a strategy similar to the MK process described in Section III D. For this approach, an injector based on a DI diesel injector would be needed. However, modifications would likely be required to achieve the very high mixing rates necessary for HCCI-like combustion.

For gasoline-type fuels, DI injectors for SI engines appear attractive. However, as HCCI research evolves (per the work described in sub-sections A-E above), it may indicate that changes in these injectors are required to meet the needs of HCCI engines. For example, partial charge stratification

appears to be an attractive method for controlling the combustion rate at high loads (Section V B) and for reducing the HC and CO emissions at light loads (Section V D). However, a different type of stratification would be required for each of these cases. Achieving the desired stratification under all operating conditions would likely require specialized HCCI injectors with spray characteristics different from those of current DI gasoline injectors. R&D will be required to adapt existing injectors or to develop advanced injectors that provide the spray characteristics desired for HCCI as indicated by this research.

H. Multi-Cylinder Effects

R&D is needed to develop intake and exhaust manifold designs for multi-cylinder engines to overcome the challenge of maintaining strict uniformity of the inlet and exhaust flows of each cylinder to assure smooth engine operation. In multi-cylinder engines, manifold wave dynamics can cause small differences in the amount of hot residual combustion products remaining and the amount of fresh charge delivered to the various cylinders (see Section IV D). In conventional SI or CIDI engines, these small differences between cylinders do not significantly impact the combustion. However, ignition in HCCI engines is very sensitive to small changes in compressed-charge temperature, and these small differences can lead to significant cylinder-to-cylinder variation in combustion timing. R&D will be required to develop manifold designs that minimize this problem over the load-speed map and to develop sensors and control systems to maintain uniform combustion between cylinders.

I. Combustion Modeling

R&D is needed to develop computational fluid dynamics (CFD) and combustion models for HCCI engines to overcome the challenge of rapidly and inexpensively evaluating engine geometry and combustion system designs. Combustion modeling is central to the development of practical HCCI engine combustion systems and control methods. Chemical-kinetic modeling and kinetic modeling combined with traditional engine CFD models such as Kiva have already been used with reasonable success to investigate some aspects of HCCI [4,5,11,16]. (Also see Sections IV A & C.) In addition, initial efforts are underway to apply advanced turbulence modeling techniques to some details of HCCI combustion, as discussed in Section IV B. However, considerably more development and testing of predictive numerical models will be required to advance the HCCI concept. Efforts are needed in three main areas: chemical-kinetic mechanisms, CFD model development and submodels development (turbulence, sprays and vaporization).

Chemical Kinetics: Kinetics models for primary, surrogate fuels such as iso-octane, n-heptane, and propane are well developed and have already proven valuable for HCCI investigations. However, kinetic mechanisms for surrogate fuels that are computationally tractable yet accurately capture the autoignition characteristics of real fuels, such as gasoline and diesel fuel, under HCCI conditions need to be developed.

CFD Model Improvements: Understanding and controlling partial charge stratification (both mixture and temperature) will likely play a key role in the development of a practical HCCI engine. Accurate CFD models are required to capture the manifold and in-cylinder mixing processes used to produce these charge stratifications. Models must have sufficient temporal and spatial resolution to resolve the transient mixing and boundary layer effects. The CFD models must also be compatible with simultaneous solution of reduced-mechanism, chemical-kinetic models and submodels for sprays, and they must incorporate adequate turbulence submodels.

Submodel Development: Both port fuel injection and various direct-injection schemes are applicable to HCCI engines. Spray and other submodels are required that reproduce the fuel dispersion, vaporization, and mixing produced by these injectors. Turbulent mixing is central to all aspects of mixing and partial charge stratification, and improved turbulence models should be incorporated into the CFD models. In addition, the application of advanced turbulence concepts, such as One-Dimensional Turbulence (ODT) and Large Eddy Simulation (LES), to in-cylinder processes in HCCI engines should be further explored.

SECTION VI. CONCLUDING REMARKS

The PNGV has identified HCCI as a high-risk, long-term alternative technology deserving of increased R&D support. A high-efficiency, gasoline-fueled HCCI engine represents a major step beyond SIDI engines for light-duty vehicles. HCCI engines have the potential to match or exceed the efficiency of diesel-fueled CIDI engines without the major challenge of NO_x and PM emission control or a major impact on fuel-refining capability. Also, HCCI engines would probably cost less than CIDI engines because HCCI engines would likely use lower-pressure fuel-injection equipment, and the combustion characteristics of HCCI would potentially enable the use of emission control devices that depend less on scarce and expensive precious metals. In addition, for heavy-duty vehicles, successful development of the diesel-fueled HCCI engine is an important alternative strategy in the event that CIDI engines cannot achieve future NO_x and PM emissions standards.

The DOE believes that university and industry involvement is essential to carrying out future HCCI R&D activities. The Department anticipates this involvement will include industry review of government-funded projects and cost-shared funding of new projects. DOE will reduce its role as the fundamentals of HCCI become clear and as industry nears the point of commercializing this promising technology. In the interim, the funding DOE has requested for HCCI engine research and development will assist in only resolving the highest risk technical issues, and ultimately R&D will accelerate the introduction of HCCI engines and realization of their potential to reduce petroleum use in the transportation sector.

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List of Acronyms

4SDI = Four-Stroke Direct Injection

A/D = Analog/Digital

AR = Active Radical

BES/CSD = Basic Energy Sciences/Chemical Sciences Division

CARAT = Cooperative Automotive Research for Advanced Technology

CFD = Computational Fluid Dynamics

CHEMKIN = Chemical Kinetics rate code

CI = Compression-Ignition

CIDI= Compression-Ignition, Direct-Injection (an advanced version of the commonly known diesel engine.)

CO = Carbon Monoxide

CPU = Central Processing Unit

CRADA = Cooperative Research and Development Agreement

DI = Direct-Injection

DME = Dimethyl Ether

DNS = Direct Numerical Simulation

EERE = Department of Energy's Office of Energy Efficiency and Renewable Energy

EGR = Exhaust Gas Recirculation

EPA = Environmental Protection Agency

H₂O₂ = Hydrogen Peroxide

HC = Hydrocarbons

HCCI = Homogeneous Charge Compression Ignition

HCT = Hydrodynamics, Combustion, and Transport (modeling code)

IC = Internal Combustion

IMEP = Integrated Mean Effective Pressure (a measure of the work produced by combustion)

Kiva = (a computational fluid dynamics modeling code)

LDRD = Laboratory Directed Research and Development

LES = Large Eddy Simulation

LLNL = Lawrence Livermore National Laboratory

LVDT = Linear Variable Differential Transformer

MK = Modulated Kinetics

NO_x = Nitrogen Oxides

NRC = National Research Council

ODT = One Dimensional Turbulence

OH = Hydroxyl

OTT = Office of Transportation Technologies

PFI = Port Fuel Injection

PM = Particulate Matter

PNGV = Partnership for a New Generation of Vehicles

PWM = Pulse Width Modulation

R&D = Research and Development

SCCI = (partially) Stratified Charge Compression Ignition

SI = Spark-Ignition

SNL/CRF = Sandia National Laboratories' Combustion Research Facility

TDC = Top Dead Center

TDI = Turbocharged Direct Injection

UCB = University of California at Berkeley

VCR = Variable Compression Ratio

VVT = Variable Valve Timing