Final Report for EERE Project: **DE-EE0008478**

Title of Project:	**Co-optimized Mixed-Mode Engine and Fuel Demonstrator for Improved Fuel Economy while Meeting Emissions Requirements**

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Executive Summary

Progressively increasing regulatory demands on fuel economy and future global emission standards have led to a focus on advanced engine development to improve overall engine efficiency and fulfill emissions requirements. Low temperature combustion (LTC) and gasoline compression ignition (GCI) are two promising technologies to achieve these goals and have the advantage of using existing refinery infrastructure and subsequent economies of scale for a robust energy supply. By applying spark ignition (SI) for cold start, LTC for low load operations, and GCI for medium to high load operations, a multimode GCI engine has been developed and demonstrated, and the fuel formulation was co-optimized to maximize fuel economy improvement potential while also maintaining emissions standards.

The overall objective of this project was to develop and demonstrate an advanced multimode GCI engine with co-optimized fuels capable of achieving a 15% improvement in fuel consumption versus a production SI engine over a simulated Federal Test Procedure (FTP)-75 cycle while meeting Low-Emission Vehicle III (LEV III) – ultra-low emission vehicle 70 (ULEV70) emission targets.

To achieve the goals of this work, the project was conducted in three phases: Engineering Design, Development, and Validation. A joint experimental and computational approach was used. More specifically, a production 2.2 L diesel compression-ignition engine was modified to run multiple combustion modes. A rapid-prototype engine controller was developed and integrated with the engine. Engine testing and simulation were then conducted to explore the operating range of each combustion mode, and develop combustion strategies for both steady state and transient operations. Finally, engine performance was confirmed in engine dyno testing, and the fuel economy improvement was determined by running 1D FTP-75 cycle simulations with the engine test data.

Key achievements and contributions from this work are as follows. A multimode GCI engine as proposed was successfully developed. Two key technologies were identified: 1) dual continuously variable valve duration (CVVD) and continuously variable valve timing (CVVT) systems for both intake and exhaust valvetrain, and 2) high pressure gasoline fuel injection system. The feasibility of this multimode GCI engine was confirmed in engine testing, and fuel economy improvement of 18% and higher over the baseline SI engine was demonstrated in FTP-75 vehicle drive cycle simulations. Aftertreatment systems for lean gasoline multimode engine were proposed to meet both ULEV70 and SULEV30 standards. In addition, a database of fuel-spray characteristics and ignition delays for six different fuels utilizing constant-volume combustion chamber testing was created. Additionally, a real-fuel model and CFD model for this multimode GCI engine was developed and validated, and will be shared with the Co-Optima team. Table 1 shows the comparison of major goals and accomplishments.

Table 1: Comparison of project major goals and achievements

Goal	Accomplishment
Multimode engine control development	Control logic for sensors, actuators, and in-cylinder feedback controls were developed and used for engine testing. The in-cylinder feedback controls appeared to be critical in extending the operating range of each mode, as well as mode switching.
Multimode engine development	A multimode GCI engine was built with a high-pressure gasoline fuel system and production-level CVVD and CVVD systems for both intake and exhaust valves. All SI/LTC/GCI combustion modes were demonstrated and tested.
Demonstration of steady state multimode operation	Operating ranges of LTC and GCI modes were explored and corresponding combustion strategies were developed.
Demonstration of combustion mode switching	Combustion mode switching was successfully demonstrated with a ramp rate of 1bar BMEP/sec from 1-12bar BMEP at three different engine speeds; 1500, 2000, and 3000rpm.
Power target of at least 150hp (BMEP 15bar from 2000 to 4500rpm)	BMEP 15-20bar was demonstrated in engine test for engine speed of 2000-3000rpm. Without a 1000+ bar gasoline fuel pump, the higher load/speed conditions with BMEP >15bar and engine speed>3000bar were not tested in the engine. As result, the rated condition (200hp) of 4500rpm/18bar BMEP was evaluated in CFD simulations.
Fuel formulation for multimode GCI engine	Nine different fuel formulations were tested at different engine operating conditions. A potential fuel was determined as a biofuel blend of 75% RON60+25% iso-butanol (IB25), which has about 14% reduction in life-cycle GHG emissions over AKI87 E10 fuel.
Real fuel model development	A real fuel model capable of capturing both fuel physical properties and chemical kinetics was developed and validated for RON 60-90 and biofuel blends with ethanol and iso-butanol.
3D CFD multimode combustion model development	The CFD model for this multimode GCI engine was built and validated at different modes (SI, LTC and GCI) and loads, as well as for six different fuels.
Create spray and combustion database for high pressure direction injection for different fuels	Six different fuels (RON 60, 70, 80 and 90, and two biofuel blends) were tested in a spray chamber at different charge gas conditions representing engine low, medium, and high-load operation. Spray characteristics and ignition delay time were determined and used for CFD model validation.
FTP-75 driving cycle simulation to compare fuel economy (target 15% improvement) while meeting emission standards	The multimode GCI engine with co-optimized fuel- IB25 was confirmed to have an 18% fuel economy improvement over the baseline SI engine with a potential gain of 30-76% using engine downsizing and hybridization.
Aftertreatment development	Two aftertreatment systems were proposed per engine test data to meet both ULEV70 and SULEV30 emissions standards.

A summary of the outcome of this research at a high level of problem area is provided below.

1) *How does the research add to understanding of the area investigated?*

- This research provided a practical approach to realize the benefits of high efficiency and low emissions from gasoline compression ignition combustion (GCI) and low temperature combustion (LTC) by using advanced high-pressure fuel system and production-level CVVD and CVVT systems for both intake and exhaust. These valve systems allow changing valve duration and timing in real time, enabling low temperature combustion phasing control on the fly and assisting in smooth combustion mode switching. This research also supports understanding of fuel formations that are more suitable for these advanced combustion concepts.

2) *What is the technical effectiveness and economic feasibility of the methods or techniques investigated or demonstrated?*

- The CVVD & CVVT systems employed are used in Hyundai production engines since 2019, thus, it is technologically and economically practical for mainstream adoption. The high-pressure gasoline fuel injection system, however, needs additional development and validation before it can be applied in production engines.

3) *How is the project of benefit to the public?*

- The practical demonstrator developed in this program has shown the potential of much improved fuel economy while meeting current and future emissions regulations and is particularly viable for hybrid vehicle applications. The corresponding technologies and strategies presented could potentially be introduced into current production engines to reduce fuel consumption.

1 Introduction and Project Objectives

Current public concerns surrounding environmental conservation, energy demand and sustainability have led to more stringent emissions regulations as well as increased investment in renewable or alternative fuels. For the automotive transportation sector, vehicle electrification appears to be one of the promising potential tactics to meet these two ends by reducing on-road emissions and using green electricity generated by solar, wind, hydroelectric, nuclear, etc. Presently almost every automaker has been marketing itself as accelerating the timeline for electric vehicles and pushing towards the electric future. However, the world is not yet ready for this massive transition; there are many challenges to overcome, such as affordable and reliable green energy, charging infrastructures, range anxiety, and reliance on rare earth materials. It is also still debatable to go with all electric vehicles [1]. Indeed, the sustainability of the global transport sector is not likely to be solidified without further improvements in internal combustion engines [1, 2]. Furthermore, there is still significant room for improved efficiency and reduced exhaust emissions of internal combustion engines [3].

One of the advanced engine combustion concepts is LTC, or homogeneous charge compression ignition (HCCI). It has the combined benefits of low nitrogen oxides (NO_x) and soot emissions like a spark-ignited gasoline engine utilizing a three-way catalyst, and the high efficiency of a compression-ignition (CI) diesel engine. In LTC mode, fuel is injected very early so that the air-fuel mixture is well mixed prior to autoignition. Through mixture dilution with EGR and/or air, combustion temperatures are low enough to significantly reduce NOx formation. Additionally, soot emissions are minimized through premixed and lean combustion. The challenge is to have controllable LTC over a sizable operating range with acceptable combustion stability and a satisfactory maximum pressure rise rate (MPPR) level. Several different methods have been developed and have showed promising results [4-6], however it is challenging to implement in production engines.

GCI is another promising approach to gaining diesel-like high brake-thermal efficiency while reducing NO_x and soot emissions through lean operation with high compression ratios. GCI here references to gasoline compression-ignition combustion with all fuel injections taking place late in the compression stroke (near firing TDC) or even after, burning fuel as in a diesel engine. It includes partially premixed compression ignition (PPCI) and mixing controlled compression ignition (MCCI). Gasoline fuel has higher volatility and lower reactivity or higher resistance to autoignition when compared to diesel fuel, leading to better mixing of fuel and air before combustion, and in turn, reduced soot emissions [7]. NO_x emissions can be reduced through lean or diluted combustion. The challenge is operation at low and high loads. The long ignition delay of gasoline fuels can lead to large cycle-to-cycle variations and even misfire at low loads with low boost and ultra-lean conditions, and too-rapid combustion and high pressure rise rate at high loads. At high speed and high load conditions, a high-pressure gasoline fuel injection system is also needed to improve fuel atomization, vaporization, and mixing for reducing soot emissions [8].

From this perspective, a multimode production-intent GCI engine was proposed, developed, and studied. This multimode GCI engine can operate in three different combustion modes, including SI for cold start, LTC for low load (SA-LTC), and GCI for medium to high loads, as shown in Figure 1. The gasoline blend-stock fuel specification was also co-optimized to maximize the potential of thermal efficiency improvement and emission reductions.

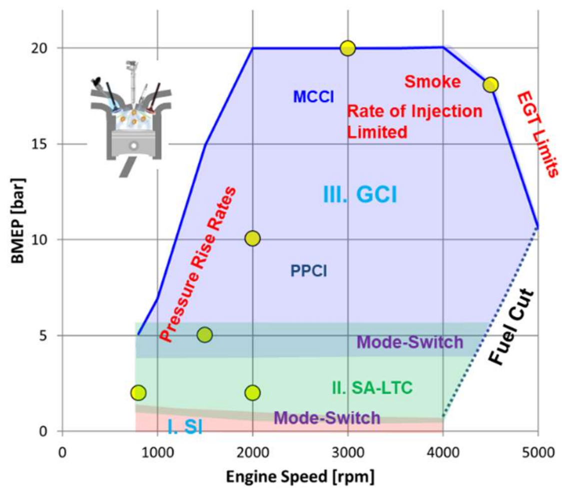

Figure 1: Schematic of multimode GCI engine map

The overall project goal is to demonstrate that such a multimode GCI engine is feasible and capable of achieving a 15% improvement in fuel economy as compared to the production SI engine over a simulated FTP75 cycle while meeting Low-Emission Vehicle III (LEV III) – ultra-low emission vehicle 70 (ULEV70) targets. It aims to overcome challenges and shortcomings of advanced GCI engines such as cold start, efficient low load operation, emissions at high load, mode-switching, and a high specific power output target of at least 150hp.

The major objectives are as follows:

- Improve vehicle fuel economy by 15% over the baseline, enabled by operation in SA-LTC mode for part load and GCI (indicated mean effective pressure [IMEP] >5 bar) over most of the engine operating range, as validated by engine dynamometer testing and vehicle simulation.
- Attain a power target of at least 150 hp (15 bar BMEP) with a 2.2 L engine via a variable-inlet-compressor-enabled highly diluted charge system ($\lambda' = 1.8$) over the full load operating range from 1,500 rpm to 4,500 rpm (targeting IMEP = 20 bar from 2,000 rpm to 3,500 rpm and 200 hp at 4,500 rpm).

- Achieve LEV III (ULEV70) emission targets or lower via robust, ultra-low cold-start emissions enabled by port fuel injection–direct injection SI mode for cold start and catalyst heating and lean gasoline selective catalytic reduction for LTC mode operation.
- Demonstrate multimode combustion control utilizing a multiple-input, multiple-output controller and cylinder pressure feedback, as well as in-cylinder conditions estimation.
- Validate computational fluid dynamics (CFD) models incorporating advanced physics-based fuel surrogate models for thermo–physical properties and reaction kinetics.
- Populate a spray and combustion database with a high-pressure direct injection system with high-reactivity gasoline (60–90 research octane number [RON]) under thermodynamic GCI and homogeneous-charge compression-ignition (LTC) conditions.
- Produce a CFD mesh and models for spray and engine data, and share them with the Co-Optimization of Fuels and Engines (Co-Optima) team.

The developed multimode GCI engine has an advanced high-pressure fuel system, advanced engine controls, and variable-inlet compressor turbocharger, as well as a cooled exhaust gas recirculation (EGR) system. Different fuel formulations were developed and tested to determine the optimal fuel for this multimode combustion engine. The engine has production-level dual CVVD and CVVT systems on both intake and exhaust that enable negative valve overlap (NVO) to trap residuals for LTC mode operation up to 5 bar brake mean effective pressure (BMEP). The SI mode is utilized in both spark-assisted (SA) LTC and cold start to improve combustion stability, ignition, and startability.

2 Technical Approaches

2.1 Overview

Figure 2 shows the general technical approach used in this program. At first, a technical specification was developed for the 2.2 L engine. The specification established the overall engine targets for fuel economy and performance, as well as boundary conditions for a set of points that represent the engine's overall operation. These points were then used in a 1D air system model to determine the optimal turbocharger specification and to set up the 3D combustion model and optical continuously variable experiments. A matrix of four gasoline blend stocks (RON 60, 70, 80, and 90) was selected for development of a real fuel chemical mechanism and fuel properties model. The fuel model was validated with experimental data and was used in the 3D combustion code to simulate discrete combustion modes of SI, SA-LTC, and MCCI combustion.

Meanwhile, a production 2.2 L diesel compression ignition engine was modified to run multiple modes of combustion. A rapid-prototyping engine controller was developed using Matlab–Simulink model-based code and integrated with the engine. Engine testing was then conducted to explore the operating range of each combustion mode. Finally, 1D vehicle FTP-75 cycle simulation was conducted by using the engine test data.

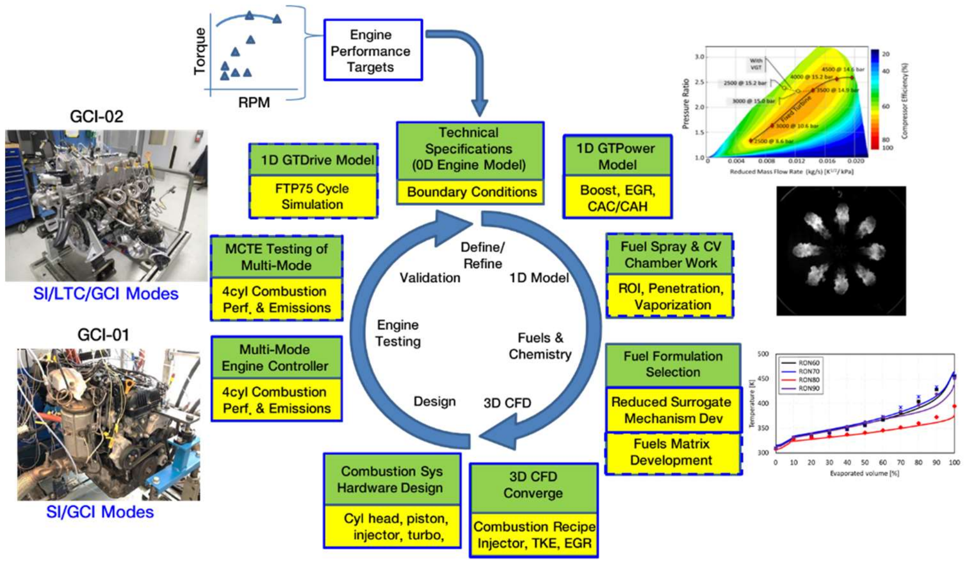

Figure 2: Co-optimized engine development approach. CAH = charge air heater; CAC = charge air cooler; CV = continuously variable; 0D = zero-dimensional; 1D = one-dimensional; 3D = three-dimensional; ROI = rate of injection; MCTE = multi-cylinder test engine; TKE = turbulence kinetic energy; cyl = cylinder.

HATCI worked with Michigan Technological University (MTU) and Philips 66 for development of a detailed fuel mechanism, validation and engine modeling in CFD, advanced controls algorithm development, and engine testing with nine different fuels, including alcohol blends. Philips 66 worked on fuel formulation development, creating gasoline-like fuels with desired physical and chemical properties for multimode combustion. These fuel formulations were tested at MTU. The MTU team also conducted 3D CFD modeling over the SI, SA-LTC, and GCI modes for different fuels. HATCI developed the overall engine hardware, multimode steady-state engine testing, mode switching demonstration, engine maps, and a 1D vehicle simulation over the FTP-75 cycle.

2.2 Experimental Testing

Experimental testing includes engine testing, and optical-spray and combustion vessel (S&CV) testing.

2.2.1 Engine Testing

Engine Setup

In this program, the final engine developed from this project was the 2nd generation GCI engine (GCI-02) [9]. It is a diesel-based four-cylinder 2.2L turbocharged engine equipped with CVVD & CVVT mechanisms for both intake and exhaust valvetrain. The engine has a compression ratio (CR) of 16:1, and is outfitted with both port and direct fuel injection systems, both high and low pressure cooled EGR loops, and a spark-ignition system. The high-pressure gasoline fuel system, developed by Hyundai Motor Europe Technical Center, consists of an engine-oil lubricated injection pump, common rail injection, and modified diesel injectors.

Table 2 summarizes the basic engine specifications. Figure 3 shows the schematic diagram of the engine layout.

Table 2. Engine Specification (GCI-02)

Engine	GCI-02
Displacement [L]	2.2 (4-Cylinder)
Bore [mm]	85.4
Compression Ratio [-]	16
Piston	Stepped-Lip Bowl
Fuel Injection	1. Port Fuel Injection - 5bar Max 2. Direct Injection - 1800bar Max
Valve System	CVVD & CVVT for Intake and Exhaust
Turbocharger	Variable Inlet geometry compressor & Variable Geometry Turbine
EGR	High/Low Pressure Cooled EGR Loops

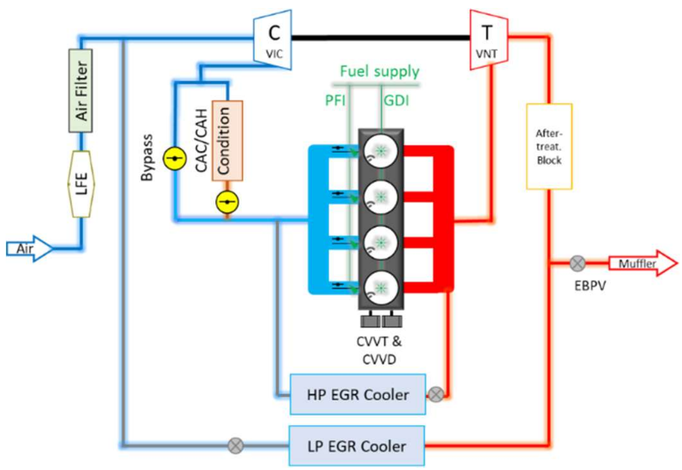

Figure 3: Engine schematic layout

The gasoline direct injection (DI) system was designed for up to 1800bar injection pressure [8], however this version of the high-pressure fuel system was not ready for engine testing. Instead a similar 1000bar fuel system was used for this project.

The GCI-02 engine is capable of running multimode combustion with intention of spark ignition for cold start, LTC for low load, and GCI for mid to high loads. The LTC here refers to HCCI combustion mode with early fuel injection - before or during intake stroke, and HCCI-like combustion with the majority of fuel injected early and one small injection (up to 20% of total fuel mass) around firing TDC [9]. GCI mode with all fuel injections near firing TDC typically requires higher direct injection pressure (e.g. greater than 250bar) and higher boost levels (e.g., greater than 140kPa) than LTC, to ensure sufficient fuel-air mixing, and consistent and reliable auto-ignition. In terms of combustion characteristics, LTC is a prevalently fully premixed combustion, while GCI is a partially premixed or stratified combustion, in between fully premixed and fully diffusion combustion.

To realize LTC without additional intake heating, the negative valve overlap (NVO) approach was used by advancing exhaust valve closing (EVC) and retarding intake valve opening (IVO), to trap hot combusted gases and increase in-cylinder gas temperature to promote auto-ignition of high-octane number fuels such as gasoline that has a high auto-ignition temperature. All or a majority (80%) of fuel was introduced into the cylinders during NVO or early in the intake stroke, e.g., 300° crank angle BTDC, targeting homogenous regime fuel distribution.

Regarding experimental instrumentation, measurement and data analysis, more details can be found in our previous publication [7]. In brief, all four cylinders used AVL GP15DK pressure sensors. Engine emissions were measured by using a Horiba MEXA 7500HEGR emissions bench and AVL 415S smoke meter, including total hydrocarbons (THC), carbon monoxide (CO), carbon dioxide (CO_2), oxygen (O_2), nitrogen oxides (NO_x), soot concentration and filter smoke number (FSN). An AVL PUMA 2.0 was used for low speed data acquisition, and an AVL Indi-Com was used for high speed data acquisition and analysis.

CVVD & CVVT Range

Figure 4 shows the ranges of CVVD &CVVT for both intake and exhaust valvetrain for GCI-02 engine. The adjustable valve duration ranges from 116 to 197 CAD for intake, and 125-200 CAD for exhaust. The valve phasing can be changed up to 100CAD for both intake and exhaust. In order to avoid interference with the piston, the intake valve has a fixed earliest opening point and the exhaust has a fixed latest closing point, which yields a minimum NVO of 28CAD, with the valve timing defined as 1mm lift. CVVT allows the intake valvetrain to move in the retard direction and the exhaust CVVT to move in the advance direction, resulting in maximum NVO of 228CAD.

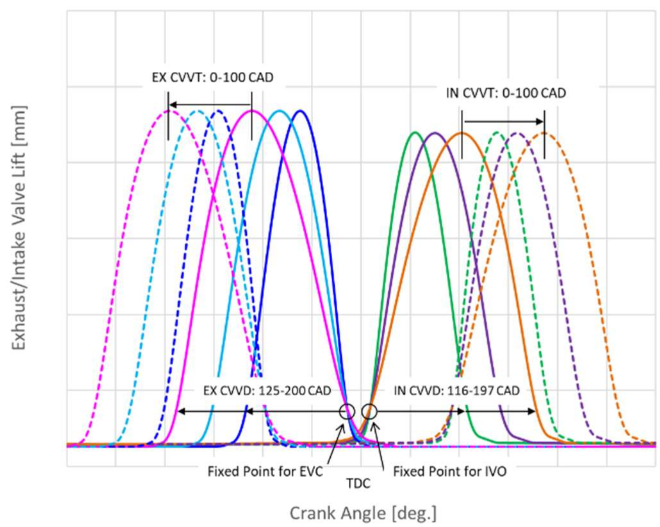

Figure 4. CVVD & CVVT range

Engine Test Conditions

The primary fuel used for this study was conventional E10 gasoline with an anti-knock index (AKI) of 87. The engine speeds and loads tested were 800-3500rpm, and 1-20bar BMEP. SI mode was used to start the engine, LTC for low load operation with BMEP up to about 7bar, and GCI for medium to high loads with BMEP from about 5 to 20bar.

For LTC operation, intake air temperature was kept around 25°C; no intake heating was applied. Fuel injection pressure was 4.5bar for PFI, and 250bar for DI.

For GCI operation, the intake air temperature was maintained at about 40°C, although higher temperatures could be used since boosted air was needed. The DI fuel pressure ranged from 250bar to about 1000bar, depending on the engine speed and load.

Data Measurement Criteria

Engine test data were taken with the following criteria:

- COV of IMEP $\leq$ 3% (4% for BMEP< 2bar)
- MPRR $\leq$ 10bar/deg.
- NO_x emissions $\leq$ 5g/kWh
- Soot emissions FSN $\leq$ 1
- Max in-cylinder peak pressure $\leq$ 180bar

Multimode Engine Control

To enable multimode engine operation, model-based combustion controllers were designed. Figure 5 shows the control architecture for each mode. This in-cylinder feedback control, including combustion phasing (CA50) and IMEP balancing across cylinders, was to be critical in extending the operating range of each mode, as shown in our publication [10]. Another critical in-cylinder feedback control was the multimode cycle-to-cycle combustion controller for the mode switching, as shown in Figure 6. More detail is discussed in the results section.

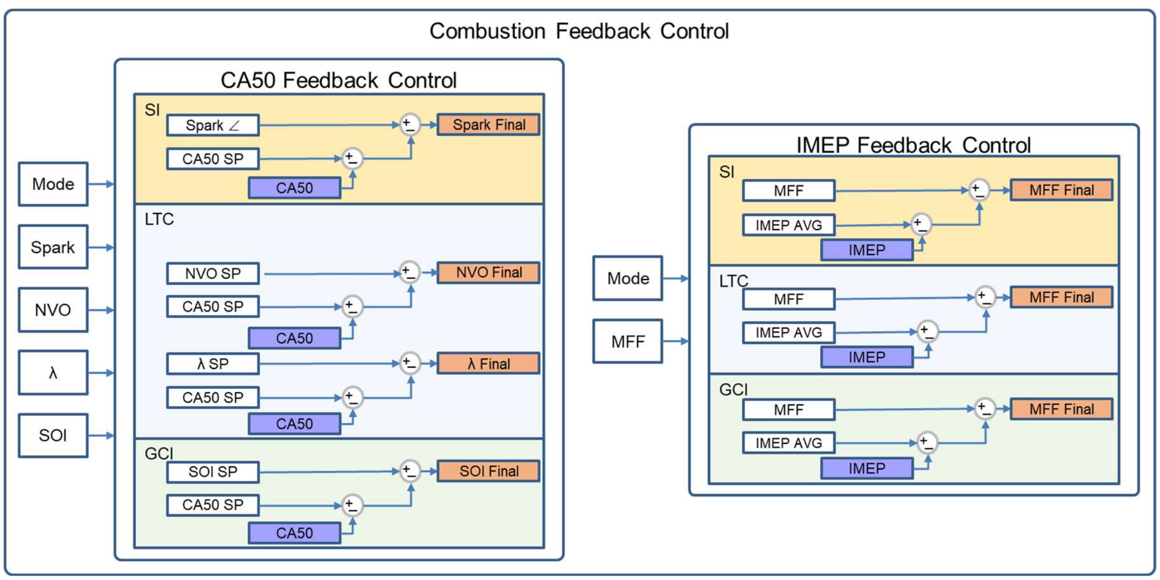

Figure 5: Model-based combustion controller

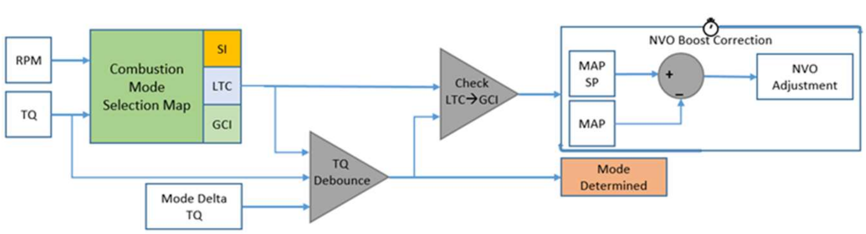

Figure 6: Multimode cycle-to-cycle combustion controller for mode switching

2.2.2 Optical Spray and Combustion Vessel Testing

MTU used its Spray and Combustion Vessel (S&CV) facility to study the spray and combustion characteristics of different fuels under direct injection GCI conditions. The testing supported fuel formulation selection efforts, data inputs for a 3D numerical model, and development of an advanced compression-ignition merit function.

Figure 7 shows the S&CV test setup. The S&CV was shown here with optical quality sapphire windows installed for imaging and lighting. A Photron Fastcam SA1.1 high-speed camera was equipped with a 60mm lens with the aperture set to F32 and capturing images at 20,000 frames per second. The high-speed optical diagnostics capture the natural luminosity of the soot oxidation of the flame and MIE scattering for hydraulic fuel injection detection. A high-intensity flash lamp was timed to illuminate the fuel injector tip for the light scattering of the liquid fuel droplets during injection and a neutral density absorptive filter was used to attenuate the high-intensity broadband light emissions during combustion. A sample image showing the natural luminosity and MIE scattering diagnostics shown in Figure 7 on the right.

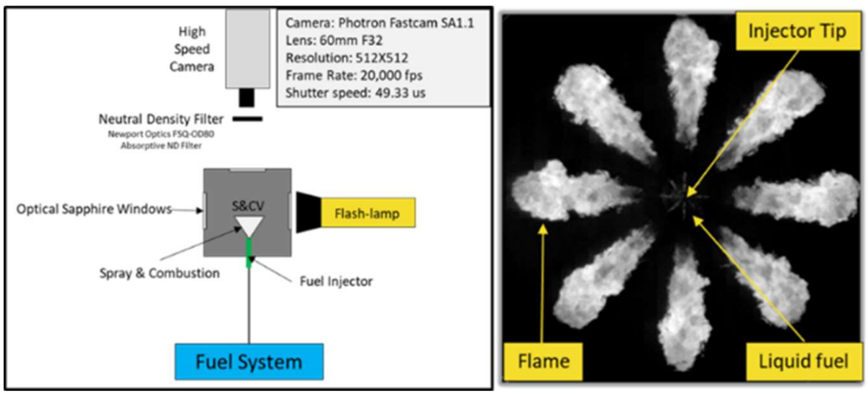

Figure 7: Left: MTU test setup including fuel system, S&CV, and high-speed natural luminosity imaging setup; Right: Sample image showing natural luminosity diagnostic capturing flame luminosity and mie scattering capturing liquid fuel injection

The images acquired during the high-speed photography were analyzed to find ignition delay at each condition. The charge gas conditions at the time of injection were chosen cooperatively between HATCI and MTU to be representative of engine operating conditions. Table 3 lists the fuel blends studied.

Table 3: Gasoline surrogates and oxygenated fuel blends

Fuels	Chemical Class (Vol%)				
	n-alkanes	iso-alkanes	cycloalkane	alkenes	aromatics
RON 60	33.4	40.6	18.7	0	7.21
RON 70	29.84	40.03	16.69	0	13.42
RON 80	23.72	40.47	16.87	13.51	5.41
RON 90	15.01	39.19	12.18	12	21.59
E36Gas	63.4% RON 60 + 36.6% Ethanol (Target RON 90/Measured 93.4)				
iB51Gas	58.8% RON 60 + 51.22% Iso-Butanol (Target RON 90/Measured 94)				

2.3 Numerical Simulations

To develop combustion strategies and determine combustion performance for different fuels at different combustion modes, a physics-based CFD model of high fidelity is needed to capture in-cylinder flow field, fuel injection and combustion accurately. It requires real fuel modeling so that both fuel physical properties and chemical kinetics of a real fuel can be well represented and simulated.

The numerical simulation model development then includes real fuel model development and CFD model validations using S&CV and engine test data.

The CFD model was initially created with MTU-KIVA-Geq-CHEMKIN code, an in-house version of KIVA code [11,12], and then re-built in Converge CFD software [13].

The code employs various physical models such as Multicomponent Surrogate Fuel Model [14-16] (to capture spray and evaporation accurately), Discrete Particle Ignition Kernel (DPIK) model [17] (to simulate the initial stages of ignition process from spark ignition to flame propagation), G-equation model [18] (a turbulent combustion model that tracks flame propagation represented by an iso-surface of a scalar). The code also includes sub-models related to drop breakup, collision and coalescence, drop deformation, wall impingement and vaporization, etc.

A hybrid primary spray break-up model that is computationally efficient as well as comprehensive enough to account for the effects of aerodynamics, liquid properties and nozzle flows was employed [19]. A droplet collision model based on the stochastic particle method [11] was used, in which the collision frequency is used to calculate the probability that a drop in one parcel will undergo a collision with a drop in another parcel, assuming all drops in each parcel behave in the same manner. Droplet deformation in terms of its distortion from sphericity is modeled using a forced, damped harmonic oscillator model, where the surface tension and viscosity of the droplet are the major properties used in the restoring force and damping terms, respectively [20]. Effects associated with spray/wall interactions, including droplet splash, film spreading due to impingement forces, and motion due to film inertia were considered in a wall film sub-model, in addition to calculations of film transport on complex surfaces with heating and vaporization of the film, and separation and re-entrainment of films at sharp corners [21]. For the turbulence calculation, the RNG k-ε model [22] was used. In the two-phase transport equations, droplets are treated as point sources and the wall film fuel flow is not resolved on the computational grid. Therefore, it is assumed that in a computational cell where droplets or wall film parcels exist, the liquid vaporizes under the prevailing mixture conditions and the vapor mixes completely with the gaseous mixture within the cell. Thus, stratification of gaseous species within a single cell are not resolved. In addition, in order to enhance computational efficiency, chemistry calculation of numerical cells is parallelized. These models have been well validated and employed in many previous works [22-25].

For NOx formation calculations, a four species (N, NO, N_2O and NO_2) and reduced 14-reaction mechanism derived from detailed GRI NOx mechanism [26] is included. For soot prediction calculations, a phenomenological soot model [27] derived from the Hiroyasu soot model that uses a competing formation and an oxidation rate formation is employed. This model utilizes acetylene (C_2H_2) as inception species for soot formation, which improves the soot prediction capabilities of the model by coupling with detailed chemistry calculations. Nagle-Strickland- Constable (NSC) was employed for soot oxidation calculations. The sooting tendency under high temperature and pressure conditions predicted by this model is in well agreement with the experiments of Sandia [27].

The final reduced chemical mechanism developed for different fuel formations has 270 species and 1229 reactions with a reasonable tradeoff between computational cost and performance.

3 Results and Findings

3.1 Low to Medium Load Operation – LTC

For operation at low to medium loads (BMEP up to ~ 7 bar), LTC was used through NVO without additional intake heating. The amount of NVO was adjusted in real time with respect to the changes in engine loads or operating conditions, thanks to the dual CVVD and CVVT mechanism for both intake and exhaust valvetrains, significantly improving LTC phasing control. Spark assist and PFI can be also used to further improve combustion stability, and double injection to create fuel stratification for reduced MPRR at medium load [10].

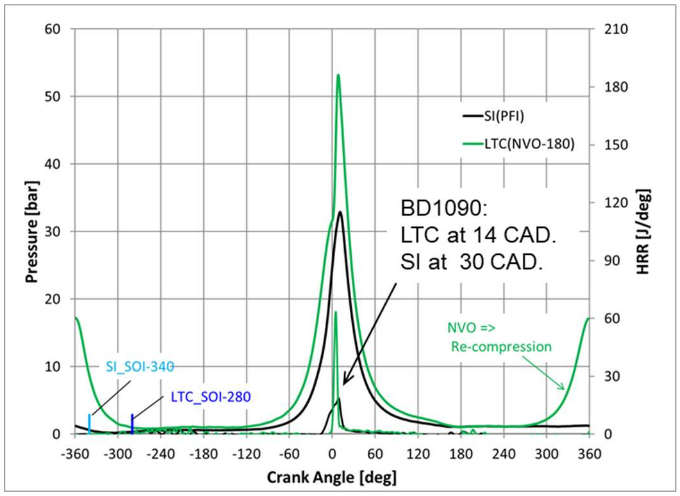

Figure 8: Combustion pressure and heat release rate for LTC (NVO-180, DI 250bar) and SI modes at 1500rpm and 2.6bar BMEP

LTC Phasing Control

Figure 8 shows a comparison of pressure trace and combustion heat-release rate between SI mode and LTC mode with the GCI-02 engine. Since LTC has an NVO of 180CAD, the re-compression process resulted from NVO can be easily seen. In comparison with SI mode, LTC shows very fast combustion with a high peak of heat release rate and a short duration, which results in better thermal efficiency, e.g. 17% ITE_{net} improvement. The diluted combustion also reduces NOx emissions by 99%, total unburnt hydrocarbon by 10%, and also possible CO reduction.

To study the combustion phasing control of LTC, the SOI timing of direct injection with 250bar fuel pressure was swept from -380 to -180 deg. $ATDC_f$, for different NVO settings (170 to 204CAD) at 1500rpm and approximately 2.6bar BMEP, as shown in Figure 9. The fuel mass flow rate was kept constant, and the throttle was fully open for all cases. The NVO reported here is symmetric NVO, that is, the retard angle of intake valve opening is the same as the advance angle of exhaust valve closing. The NVO was varied while the exhaust valve opening and intake valve closing were kept constant.

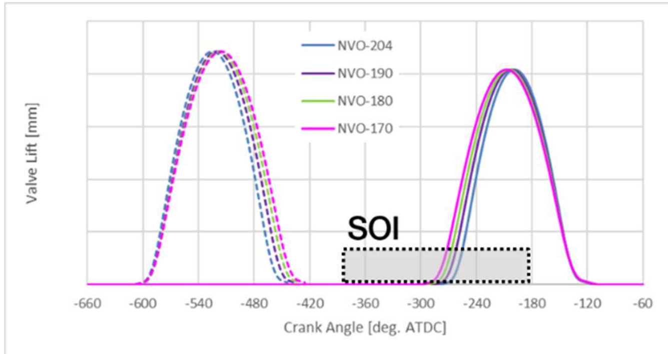

Figure 9: SOI sweep for LTC with NVOs of 170-204CAD at 1500rpm/2.6 BMEP (250bar DI)

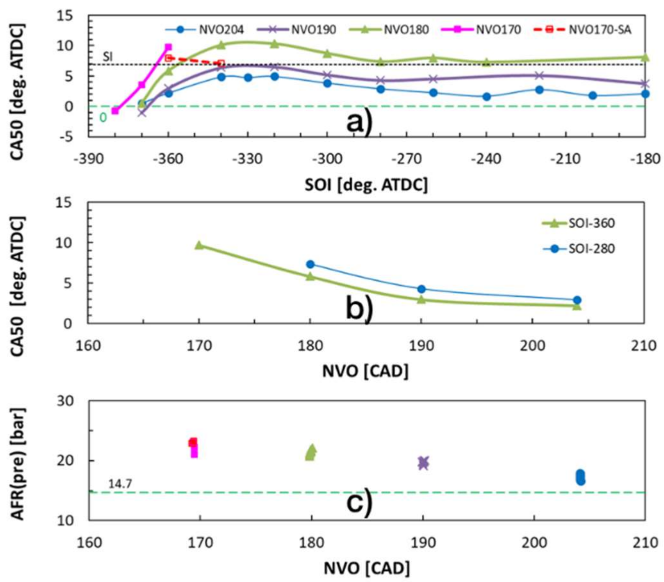

Figure 10: CA50 and AFR for LTC in Figure 9

Figure 10a) shows CA50 of LTC for different DI SOI timings with different NVO settings. NVO170-SA represents the spark assist case for NVO170. The effect of spark assist will be discussed later. The key conclusion here is that CA50 has a non-monotonic relationship with SOI timing for a given NVO, but a clear trend is observed as the SOI timing is early and between -330deg to -380deg: more advanced SOI timing means more advanced CA50. Figure 10b) replots the CA50 against NVO for two SOIs, SOI-360 and SOI-280. Different SOI affects combustion phasing slightly, but clearly, less NVO leads to retarded CA50. Therefore, NVO along with fuel injection can be used to control the combustion phasing of LTC.

Figure 10c) plots the NVO effect on overall air fuel ratio (AFR). With the NVO increased, the mixture is richened due to more trapped residuals and less fresh air entering the cylinders. But all cases were operating in overall lean conditions, with AFR higher than 14.7. Meanwhile, more NVO also indicates higher in-cylinder gas temperatures since the ratio of hot residuals to fresh air is higher, leading to even earlier and faster combustion, further explaining why NVO can be used to control the LTC phasing.

LTC Stability Improvement

To improve LTC stability, the effects of spark assist and fuel injection between PFI and DI were studied.

Figure 11 shows the spark assist effect in LTC at the low load of 1500rpm and 1.1 BMEP. The spark timing for the case with spark assist was swept from 10 to 40 deg. BTDC. Compared to the case without spark assist, the spark contributes to an earlier start of combustion, that is, CA5 taking place slightly earlier, resulting an earlier combustion phasing of CA50. The COV of IMEP was then reduced from 4.8% to 4%, while the combustion duration did not have noticeable changes. Earlier spark timing did not lead to earlier start of combustion or combustion phasing. No significant change was observed in the net ITE or emissions.

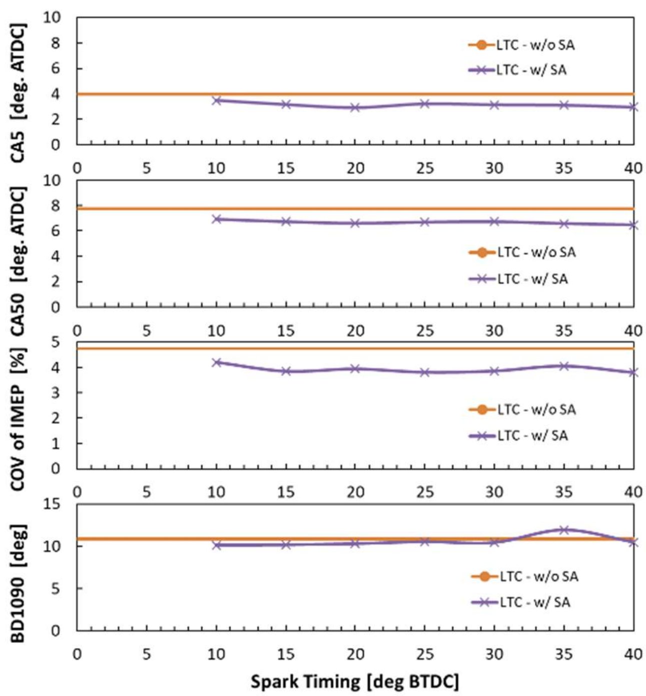

Figure 11: LTC without and with Spark Assist at 1500rpm and 1.1bar BMEP (NVO-200, PFI, SOI-250) [10]

Figure 12 compares the combustion performance between PFI and DI for LTC mode at 1500rpm and 1.1bar BMEP. The NVO was 200CAD. Spark assist with timing of 30deg $BTDC_f$ (firing) was used since it helped in reducing COV of IMEP. The SOI was varied from -360 to -180 deg. ATDC. At this low load condition, fuel injection quantity is small. Injecting such a small quantity of fuel through a DI injector that is designed for high injection pressure and high flow rate leads to large shot-to-shot fuel injection variation, hence, higher COV of IMEP compared to PFI. Additionally, the SOI timing for the DI case had to be earlier than -260deg. crank angle before TDC to have enough time for the injected fuels to be fully mixed with trapped gases, otherwise the COV of IMEP increases significantly. DI leads to slightly earlier combustion phasing and shorter combustion duration, but the higher THC emissions lead to a worse net ITE. For PFI injection timing earlier than IVO timing, that is, SOI-300 and SOI-270, injects fuel before charge flow is established and without any contact with hot residual gas, resulting in more wall wetting on the intake port and valves, and in turn, slow fuel atomization. THC emissions have shown to be high for these two early SOIs, decreasing as SOI is retarded after IVO. The net ITE increases along with THC emissions improving as SOI is retarded.

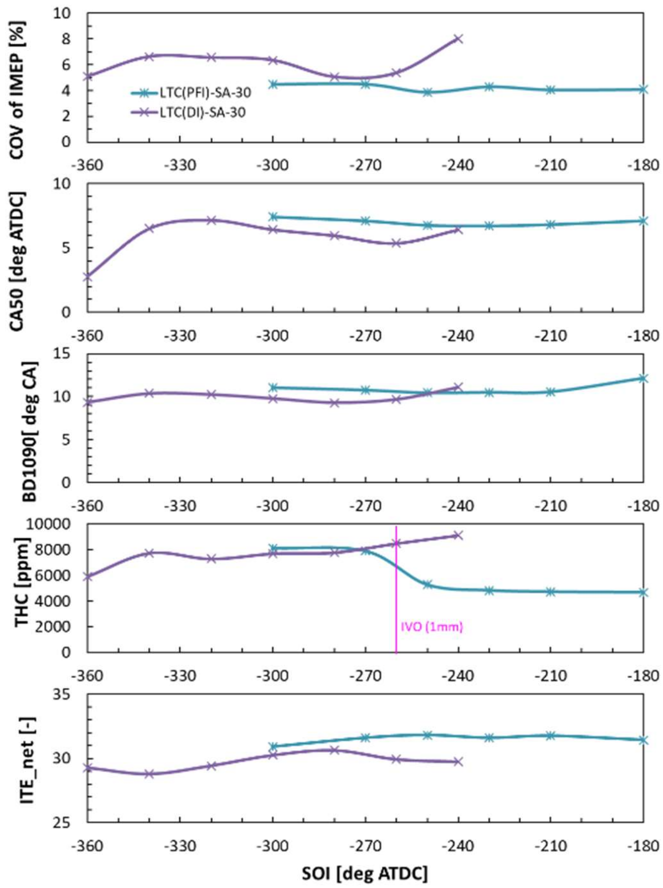

Figure 12: LTC at 1500rpm and ~1.1bar BMEP with spark assist (spark timing 30deg BTDC): PFI (4.5bar) vs. DI (250bar) [10]

The results in Figure 11 and Figure 12 indicate both spark assist and PFI can reduce the COV of IMEP and stabilize LTC resulting in extending LTC operating range.

Mitigation for High Pressure Rise Rate with LTC

As load increases, fuel flow increases. The mixture will become richer if air flow cannot increase proportionally, leading to a shorter ignition delay and higher maximum pressure rise rates (MPRR). Different approaches can be used to reduce the high MPRR including external EGR, boost, fuel stratification, etc.

Considering the high load operation with GCI, which requires high boost and late DI injections, multiple DI fuel injections were used to reduce the high MPRR for medium load operation with LTC mode.

Figure 13 shows the combustion pressure and heat release rate between single and double DI injections at 3000rpm and 3bar BMEP. Introducing a 2nd injection with fuel ratio of about 20% leads to an MPRR reduction from 5.4bar/deg to 3.9bar/deg.

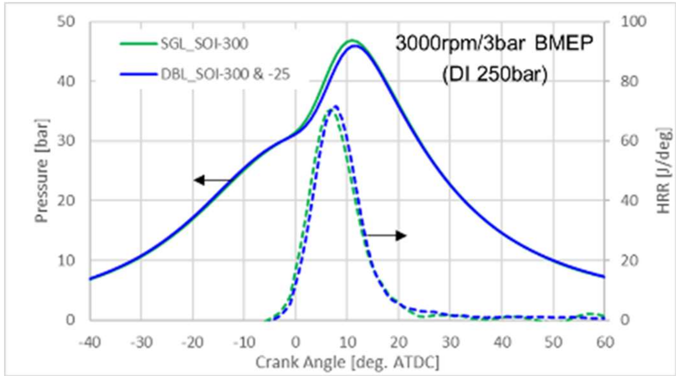

Figure 13: DI single vs. double injection at 3000rpm and 3bar BMEP

Based on parametric studies of LTC phasing control, stability improvement, and high MPRR mitigation, an LTC strategy was developed and is shown in Figure 14. Spark assist is used for low load, and can be turned off as the load increases. PFI is used for low loads to reduce the cycle-to-cycle variation. As load increases, single and early DI can be used to accommodate the need of increased fuel flow rate if any. As load increases, double DI with one late DI can be used to suppress the increasing MPRR. NVO is used to regulate the in-cylinder thermodynamic conditions to promote auto-ignition and should be reduced to suppress the unacceptable MPRR at higher loads, where in-cylinder conditions become better suited for auto-ignition.

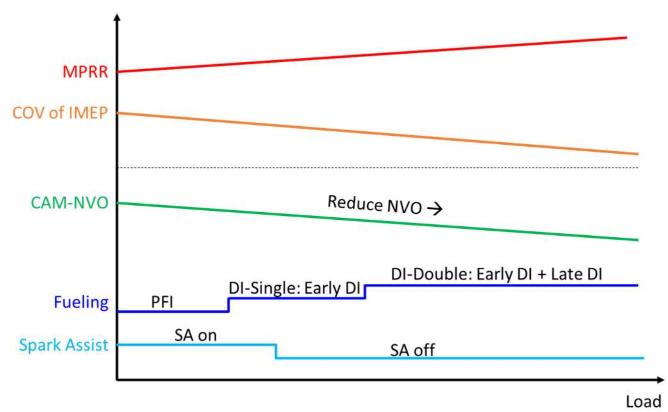

Figure 14. Proposed strategy for LTC operation from low to medium loads [10]

With the strategies in Figure 14, LTC is viable with BMEP up to about 7bar, as shown in Figure 15. That well covers the low-load range of GCI operation, which is limited at about 3bar BMEP with 3% of COV of IMEP with intake conditions of 40°C and 140kPa boost (note: Figure 15 only plots GCI with COV less than 2%). At BMEP's around 5-7bar, the intake pressure difference between LTC and GCI is only about 20kPa maximum. It indicates a higher chance of successful mode switching between LTC and GCI at these loads, considering some NVO could be used for GCI to increase in-cylinder gas temperature for compensating the negative impact on fuel air mixture auto-ignition when a lower boost is used.

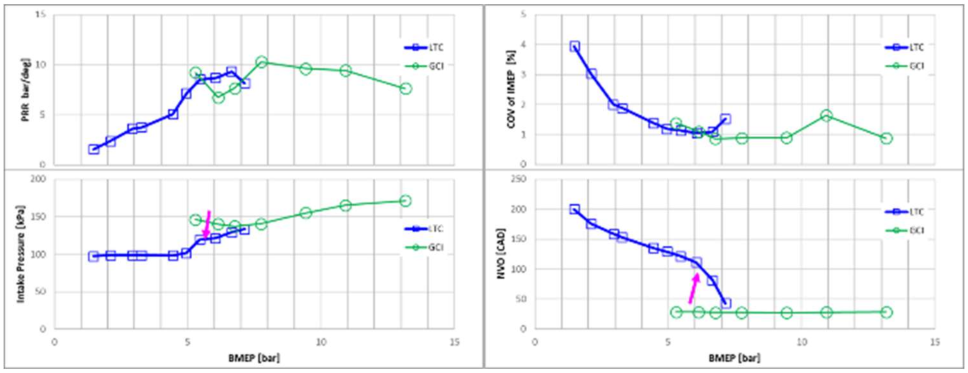

Figure 15: Load sweep at 1500rpm for LTC and GCI modes.

3.2 Medium to High Load Operation – GCI

For operation at medium to high loads (BMEP greater than 5bar), GCI was used with two late direct injections near TDC_f, pilot and main. The SOI timing was around -30 and -5 deg. $ATDC_f$ for pilot and main injections. At medium loads with BMEP around 5bar, the fuel split ratio between pilot and main can be around 60/40, to take advantage of high combustion efficiency and low emissions from PPCI. For higher loads with BMEP greater than 15bar, the fuel split ratio needs to be decreased to around 15/85 for MCCI to reduce the MPRR. More details on the GCI combustion strategy can be found in [7].

Figure 16 shows two typical GCI combustion modes, PPCI at a) 1500rpm/5bar BMEP and MCCI at b) 2000rpm/20bar BMEP. In Figure 16a), the early pilot injection along with the large quantity (approximately 60% split) leads to significant air fuel mixing. The long ignition delay at relatively low boost results in a late start of combustion that is even after the main injection starts, thus a strong and dominant premixed combustion as indicated by one peak of HRR and sharp rise of combustion pressure. In Figure 16b), the reduced pilot quantity (about 15% split) still leads to an early pilot premixed combustion due to a shorter ignition delay at a higher boost as shown by the first high peak of HRR and the fast rise of the combustion pressure before the main injection. The main injection starts around the HRR peak of premixed combustion, which is expected to quench somewhat the premixed combustion initiated by the pilot injection, and then mixing controlled combustion follows and prevails, as shown by the long diffusion flame tail end of MCCI mode extended to about 60deg $ATDC_f$.

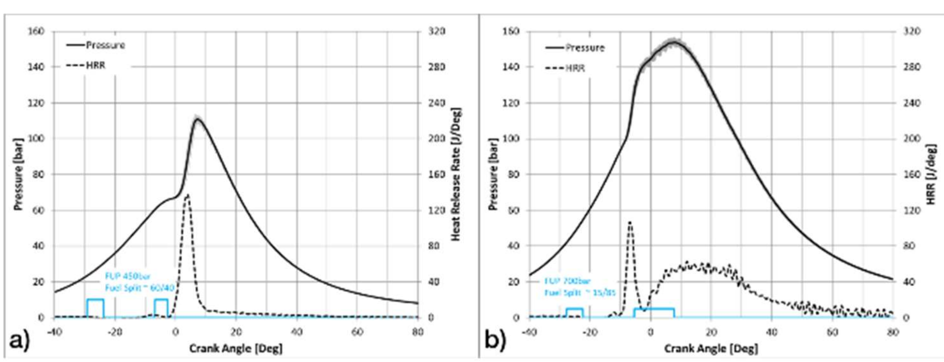

Figure 16: Combustion pressure and heat release rate for GCI at a) 1500rpm/5bar BMEP and b) 2000rpm/20bar BMEP

For higher speed/load operating conditions, a test was tried with the engine speed greater than 3500rpm and BMEP greater than 15bar. It was found to be very challenging to run the engine without the intended 1800bar fuel system, which could not be delivered at the time, due to COVID-19 mandates and a labor shortage. In addition, the available 1000bar common rail pump had cooling issues, preventing from engine testing at higher speed/load conditions.

To assess high load and high-speed operation with this multimode engine, CFD evaluation at the rated condition, 4500rpm and 18.1bar BMEP (200hp/150kW), was carried out.

As engine results indicated, combustion duration increases as the engine load and speed increase, leading to high exhaust temperature and soot emissions. The exhaust temperature is limited by the allowable turbine inlet temperature of the turbocharger used, which is 860^{0}C. Along with the criteria listed in Data Measurement Criteria section, following limits must be followed.

- Turbine inlet temperature < 860^{0}C
- Maximum cylinder pressure Pmax<180bar
- Maximum pressure rise rate MPRR<10bar/deg.

To meet the criteria above, the following three parameters were studied at the rated condition:

- Fuel injection pressure FUP (800, 1000, and 1600bar)
- Fueling strategy (timing, single and double injections)
- Boost level, i.e., air fuel ratio (AFR: 20.7 to 22.5)

To estimate the turbine inlet temperature, full cycle simulations were performed. The validated CFD model based on engine data at 2000rpm and 20bar BMEP, shown in Figure 17, was used. Table 4 lists the operating conditions for seven cases A to G, and also corresponding combustion performance. The details for each case are discussed below.

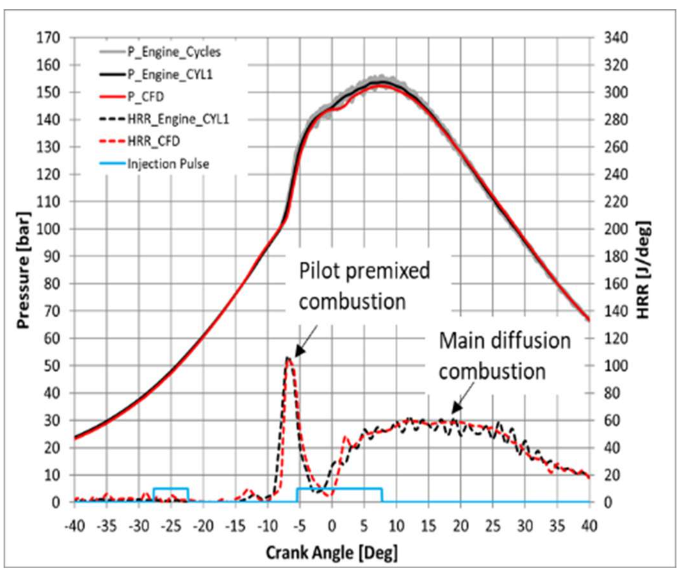

Figure 17: validated CFD model at 2000rpm/20bar BMEP (GCI)

Table 4: Summary of CFD operating conditions and results at rated condition (4500rpm/18.1bar BMEP)

Case	FUP [bar]	SOI_1 [deg, aTDC]	SOI_2 [deg, aTDC]	CA50 [deg, aTDC]	BD1090 [deg, CA]	AFR [-]	Pmax [bar]	PRR_max [bar/deg]	T_turb_in [C]	Delta soot [%] in g/kWh	Delta Nox [%] in g/kWh	Delta HC [%] in g/kWh	Delta ITE [-]
A	800	-21.5	NA	21.0	67.4	20.7	155	16.6	829	0%	0%	0%	0%
B	1000	-20	NA	16.8	53.1	20.7	166	17.7	780	-49.6%	40.8%	-74.7%	8.3%
C	1600	-19	NA	8.8	39.6	20.7	199	36.7	688	-86.0%	157.5%	-99.7%	13.1%
D	1600	-13	NA	18.3	39.2	20.7	141	9.8	759	-83.4%	32.7%	-98.0%	8.9%
E	1600	-18	-8	18.8	52.0	20.7	157	9.8	752	-49.0%	-19.5%	-85.9%	7.5%
F	1600	-18	-8	17.2	52.4	21.6	165	8.8	730	-68.5%	-4.3%	-99.1%	11.6%
G	1600	-18	-8	17.6	55.7	22.5	170	8.2	706	-45.8%	-16.1%	-90.2%	10.1%

Fuel injection pressure effect: Cases A to C with single fuel injection. The fuel injection pressures are 800, 1000, and 1600bar for Case A, B, and C, respectively. Case A with 800bar FUP has to use a long injection duration to deliver the needed fuel amount into cylinders. The long combustion duration, 67CAD for BD1090, leads to a high exhaust temperature. The turbine inlet temperature for this case is estimated to be 829°C, very close to the limit of 860°C. The MPRR already exceeds limits, 16.6bar/deg. Thus, a very small operating window is left for retarded combustion phasing to reduce MPRR; a higher fuel injection pressure is clearly needed. As the FUP is increased to 1000bar (Case B) and 1600bar (Case C), fuel atomization is improved, resulting in much more premixed combustion, more advanced combustion phasing (CA50), higher Pmax and MPRR. The fuel injection duration, combustion duration BD1090, and exhaust temperature are all decreased. Again, the MPRR is too high, and the Pmax in Case C is higher than the limit of 180bar, indicating the fueling strategy needs to be adjusted for different FUPs.

Fueling strategy effect: Cases C to E with 1600bar FUP. From Case C to Case D with single fuel injection, the start of injection (SOI) was retarded from -19 to -13 deg., aTDC. Therefore, the combustion phasing CA50 is retarded from 8.8 to 18.3 deg, ATDC. The Pmax is reduced significantly from 199bar to 141bar. The less efficient combustion resulting causes an increase in the exhaust gas temperature, but that is still far below the turbine inlet limit, 759°C vs. 860°C. The MPRR is 9.8bar/deg.,on the borderline of the limit. However, the NOx emission is higher than the baseline Case A. So in Case E, the double-injection approach with SOIs of -18 and -8deg., aTDC, was used. The fuel split for the pilot and main was 18/82. Compared to Case D, Case E has similar combustion phasing, but a longer combustion duration. NOx emissions are now reduced, about 19% lower than that of Case A, instead of 33% higher in Case D.

Boost effect: Cases E to G with double fuel injection and 1600bar FUP. The boost level for Cases E, F, and G were 2.5, 2.6, and 2.7bar, with corresponding air fuel ratios of 20.7, 21.6, and 22.5. As the mixture becomes leaner, the combustion Pmax is increasing, and the exhaust gas temperature is lower due to increased air dilution. Fueling strategy can be further tuned for a more desired Pmax and combustion performance.

These evaluation results clearly indicate that, for high speed and high load operations, a high fuel injection pressure greater than 1000bar is needed to allow multiple fuel injections, so that the engine hardware limit requirements can be met and emission reduction can be achieved. A high boost turbocharger would also help in lowering exhaust gas temperatures.

3.3 Mode Switching Demonstration at Medium Load

For mode switching from SI to LTC right after engine start, engine testing showed a very smooth transition from SI to LTC since both can be operated at similar throttle positions and the NVO can be adjusted in real time, so no detailed result is presented here.

For the mode switching between LTC and GCI, as discussed in Figure 15, mode switching at BMEP around 5bar appears be plausible. Both stationary (with the same speed/load) and transient (with varying load) mode switching were tested.

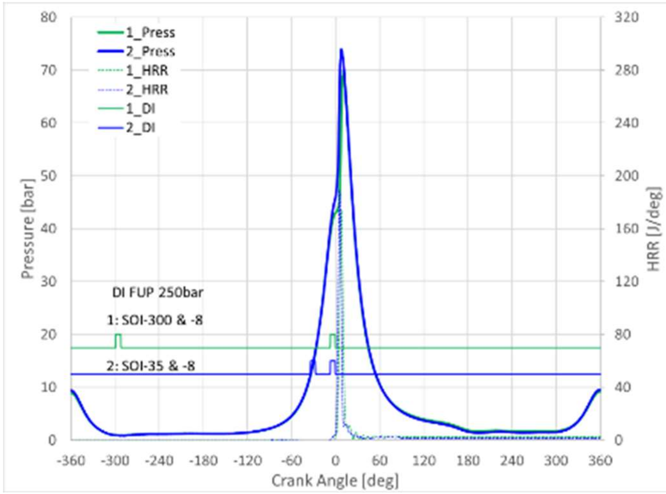

Figure 18: Stationary mode switching between LTC and GCI at 1500rpm/5bar BMEP

Figure 18 shows stationary mode switching between LTC and GCI at 1500rpm and 5bar BMEP, Case 1 in LTC mode, and Case 2 in GCI mode. The intake air temperature and pressure were 27^{0}C and 120kPa. The DI fuel pressure was 250bar. The first injection timing SOI_1 was 300deg BTDC for Case 1, and 35deg. BTDC for Case 2. The 2nd injection timing was kept the same at 8deg. BTDC for both cases. For Case 1 with LTC mode, the 2nd late injection was used to suppress the high pressure rise rate at this medium load. In other words, the only change between Case 1 and Case 2 was the SOI_1 timing. The combustion and heat release rate do not show much difference between two cases at this operating condition.

Figure 19 shows the combustion results for the two cases presented in Figure 18. As SOI timing was retarded from 300deg. to 35deg. BTDC, the combustion phasing CA50 was advanced by 3CAD. The MPRR was slightly increased from 7 to 8 bar/deg. COV of IMEP was maintained below 3%. The engine output or torque was slightly reduced, while fuel flow was decreased and SOI_1 was retarded. The decrease in fuel flow is believed to be caused by the increase of in-cylinder pressure when both injections take place at late crank angles. The ITE_net was increased by 3%, due to slightly more advanced combustion phasing and more complete combustion (less THC emissions). The NOx emission remained the same at about the limit of 5g/kWh.

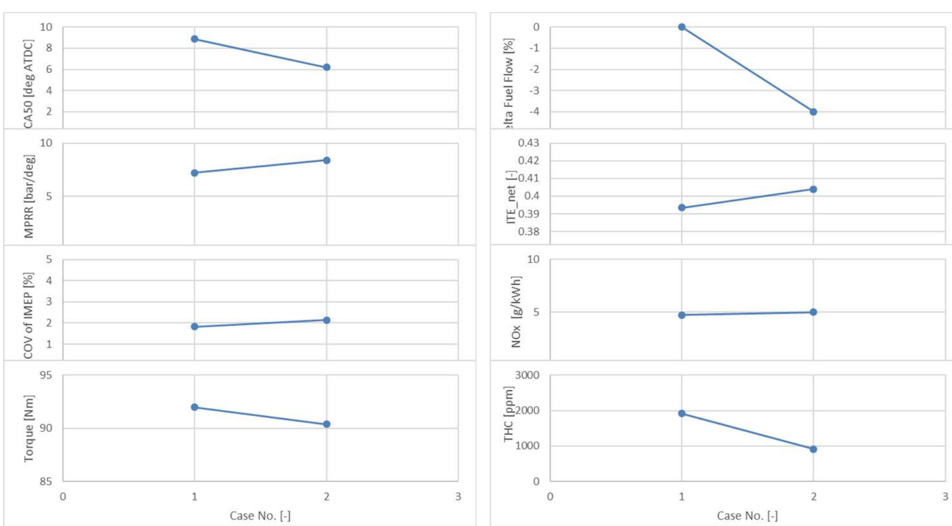

Figure 19: Combustion results for the two cases in Figure 18

It should be noted that in this case, an NVO of 108CAD was used for both cases as shown by the re-compression during gas exchange at TDC. The NVO trapped hot residuals in cylinder and increased gas temperatures. As a result, GCI combustion can be still successful even though the intake pressure was only 120kPa, compared to about 140kPa with minimum NVO (28CAD) in Figure 15.

Transient mode switching tests were successfully conducted at different engine speeds. For brevity, one case is reported here as shown in Figure 20, the load sweeps from 1bar to 12bar BMEP at a ramp rate of 1bar BMEP/second and engine speed of 2000rpm. The combustion mode was switched from LTC to GCI within the recorder time of 9sec. No IMEP drop was observed across all four cylinders. The combustion phasing CA50 was about 4deg. ATDC for low load at LTC mode, then retarded to about 12deg. ATDC for higher load at GCI mode. The MPRR did briefly exceed 10bar/deg. during the transition, at recorder time ~12.5sec where the CA50 was also advanced, ~ 7deg. ATDC, but it can be reduced below 10bar/deg. with further engine calibration.

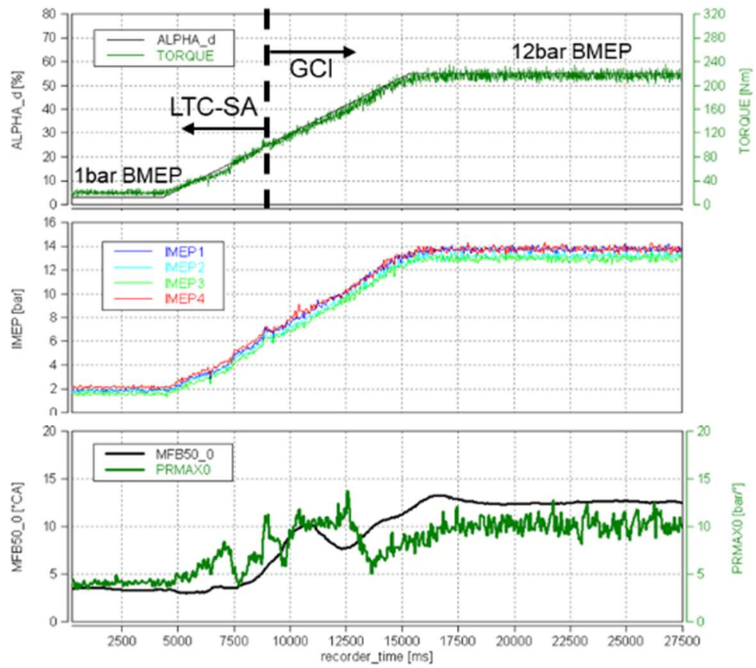

Figure 20: Load sweep with ramp rate 1bar BMEP/second at 2000rpm

Figure 21 shows the fueling injections, EVC timing, and intake boost and temperature during the load sweep shown in Figure 20. At low load with torque less than 65Nm (recorder time earlier than 7sec), only single injection with SOI around 330-300 deg. BTDC (actual SOI_1) was used. When the torque was greater than 65Nm (recorder time >7sec), an additional injection with SOI close to TDC (actual SOI_2) was introduced for suppressing the high pressure-rise rate. The EVC timing was 90deg BTDC gas exchange at ~1bar BMEP, and then retarded as engine load increased. EVC timing was 50deg. BTDC gas exchange when combustion mode was switched from LTC to GCI at recorder time~9 sec. Right after that, EVC timing was not immediately set to the most retarded position for the minimum NVO typically used for GCI mode. The reason for that was that turbo lag caused insufficient boost pressure, resulting in longer ignition delay and misfiring cycles. By keeping some NVO before boost pressure reaches the set point, then the in-cylinder gas temperature can be increased. This reduces the mixture ignition delay, offsetting the negative impact of insufficient boost pressure on auto-ignition and eliminating misfiring cycles. After the boost pressure is built up and reaches the set level, NVO can be minimized.

In this mode switching demonstration, this NVO correction for boost deficit was found to be very effective to avoid misfiring cycles and torque drop.

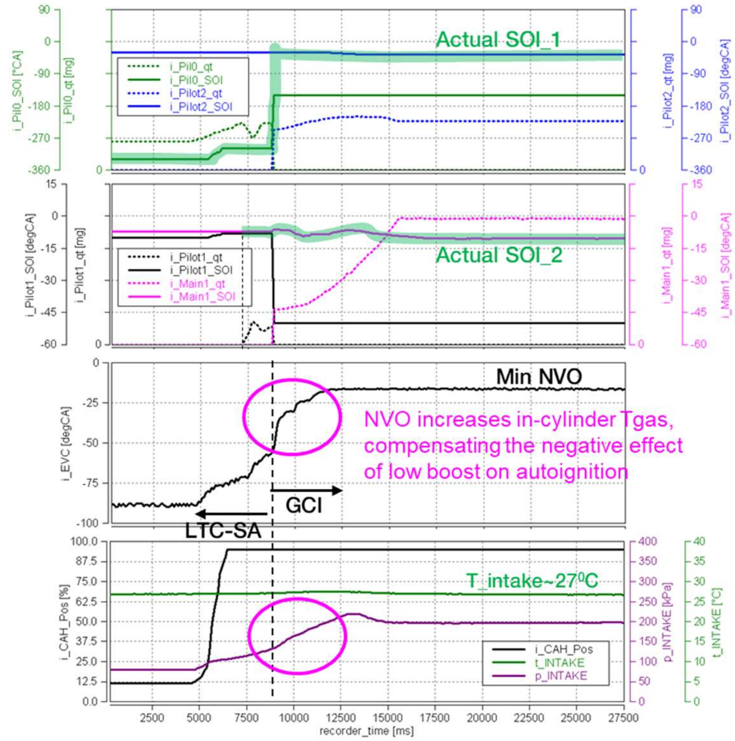

Figure 21: Fueling, EVC, and boost during load sweep in Figure 20

3.4 Fuel Co-optimization

To develop new fuels that can boost engine efficiency and reduce emissions when combined with advanced combustion techniques, nine different fuel formulations with RONs ranging from 60 to 90 were blended and tested through collaboration with Phillips 66 and Michigan Technological University (MTU). These fuels were studied with Spray and Combustion Vessel testing, CFD real fuel modeling, and engine testing. Four of these fuels were non-oxygenated gasoline refinery blend-stocks blended by a petroleum refinery at Phillips 66 with RONs from 60 to 90. Additionally, bio-renewable components of ethanol and iso-butanol were added to the base RON60 gasoline blend-stock fuel to increase the overall bio-gasoline fuel to target RONs of 80 and 90. Additionally for reference, the effect of RON91 E10 gasoline (standard US-spec pump fuel) was also included.

<u>Engine Test</u>

The engine test includes the effects of fuel reactivity on combustion characteristics, including combustion stability, rates of pressure rise, performance, and emissions to understand medium load operation and extend GCI to lower loads.

Figure 22 shows the fuel test points completed for all nine fuel formations in GCI mode. The lower RON fuels with RON<80 clearly extend the GCI low load limit down to about 1bar BMEP with COV of IMEP ≤3% due to the improved fuel reactivity.

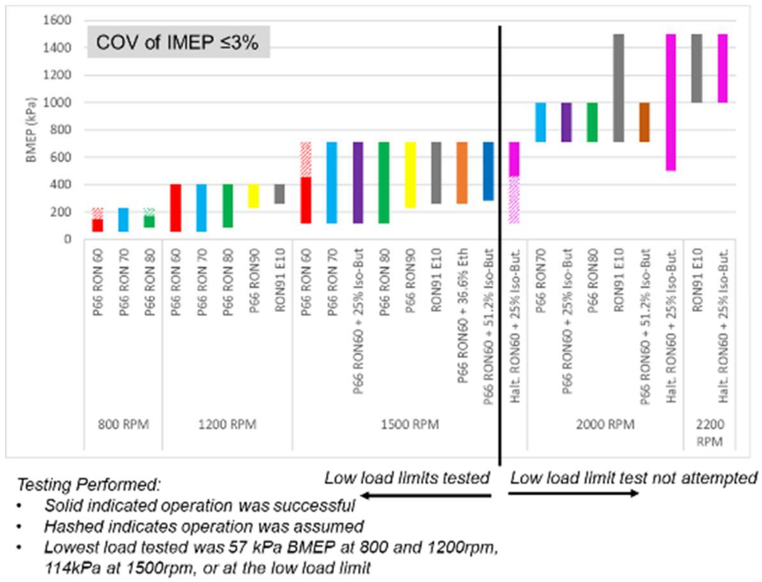

Figure 22: Fuels test points in GCI engines

Figure 23 shows the ignition delay and peak cylinder pressure for nine different fuels at 1500rpm and 4.6bar BMEP. The ignition delay time here is defined as the time duration of mass fraction burnt from 0% to 2%. Each fuel shows consistent ignition delay for different combustion phasing. Higher RON fuels have longer ignition delays. The strong grouping phenomenon – similar ignition delay for E36 (36% ethanol+64% P66 RON60), IB51 (51% iso-butanol+ 49%P66 RON60), RON91 E10, and P66 RON91, is due to their similar RON ~ 89-94. There are two distinct heat release patterns for the fuels with RON>80 and those with RON≤80 tested: single stage for RON>80 and two-stage for RON ≤80, as shown in Figure 24.

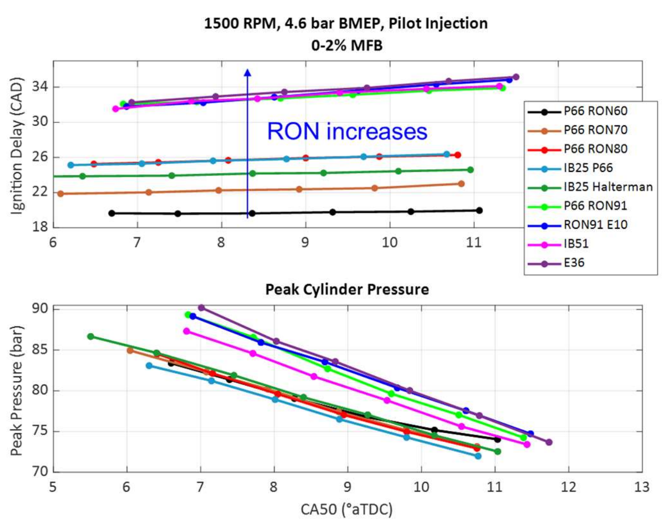

Figure 23: Ignition delay and peak cylinder pressure for different fuels at 1500rpm and 4.6bar

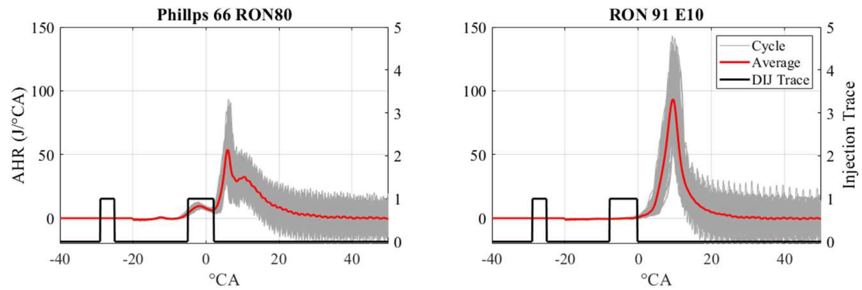

Figure 24: Heat release rate for P66 R80 and RON91 E10 at 1500rpm and 4.6bar BMEP

Among these nine different fuels, iB25 (25% iso-butanol + 75%P66 RON60) with calculated RON 77.8 appears to be the best candidate in extending GCI low load limit while maintaining good engine startability and having the benefits of reduced GHG emissions. Its better combustion performance in thermal efficiency and emissions over E10 was also confirmed at different engine operating conditions, as shown in Table 5. The relatively higher soot with IB25 in GCI mode can be reduced with a higher fuel injection pressure, since the fuel pressure used was relatively low, less than 350bar even at 10bar BMEP.

Table 5: Combustion performance comparison between E10 and iB25 at three DOE points

Parameter	1500 RPM, 5 bar BMEP		2000 RPM, 2 bar BMEP		2000 RPM, 10 bar BMEP	
Fuel	RON91 E10	IB25 Halterman	RON91 E10	IB25 Halterman	RON91 E10	IB25 Halterman
ITE Net [%]	40.8	42.5	38.4	38.8	44.4	44.4
NOx [PPM]	503	498	<25	<25	1073	586
FSN[-]	0.19	0.44	<0.01	<0.01	1.05	1.6
FUP [bar]	270	270	270	270	330	337
Mode	LTC	GCI	LTC	LTC	GCI	GCI

Spray and Combustion Vessel Test

Figure 25 provides results from S&CV tests to compare RON60 and RON90 at three different charge gas densities. The figure clearly shows that increasing density decreases ignition delay, and RON 60 has shorter ignition delay than RON90.

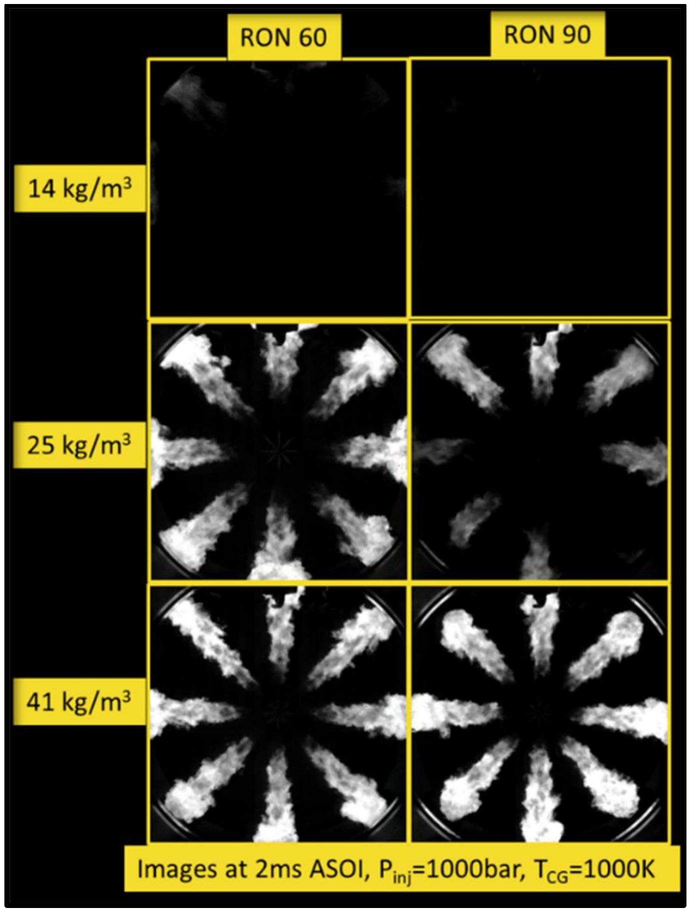

Figure 25: Sample images chosen for RON 60 & 90 gasolines at 2ms after the start of injection at each condition demonstrate the effect of charge gas density on ignition delay

Results from this work were used for the CFD calibration and validation studies. Additionally details of the ignition delay and combustion rates fed into the merit function as reactivity factors.

3.5 CFD Modeling

Distillation profile

Figure 26 shows the distillation profiles of the surrogate fuels compared to those of experiment data. The fuel surrogate model shows a good agreement with the measurements for the distillation characteristics. However, the simulation under-predicts the distillation temperature for the evaporated volume of 60 to 80 % for RON 60, 70 and 90.

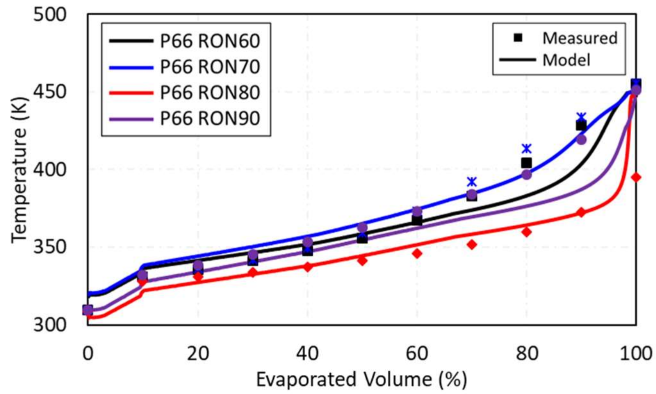

Figure 26: Distillation profile comparison between fuel surrogate model and experimental measurement for different fuel.

S&CV Simulations

Table 6: S&CV operating conditions for CFD model validation

CVCC Conditions		
	Case1	Case2
Chamber T [K]	1100	900
Density [kg/m^3]	41	14
Inj. Pressure [bar]	1000	400
O_2 [%]	17	17

Table 6 lists the two S&CV operating conditions used to validate CFD spray and real fuel models. Figure 27 shows the CFD calculated ignition delay times compared to measurement results. Simulation captures the nature of the experiments; Ignition delay for the fuels increases with RON number, and RON 60 shows the shortest ignition delay time and ethanol blend shows the longest ignition delay time.

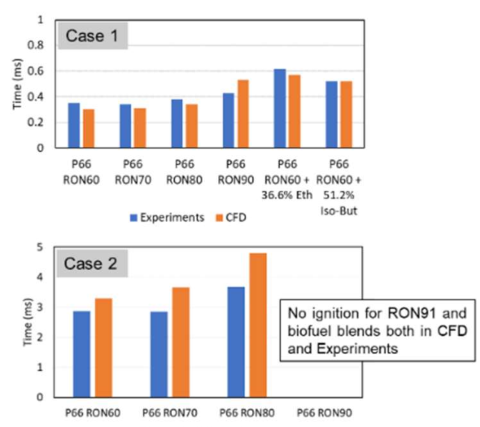

Figure 27: Ignition delay comparison between CFD and S&CV measurement for the two cases in Table 6

Engine Simulations

For the engine CFD validation, the six fuels listed in Table 3 were simulated at 1500rpm/IMEP$_{net}$ 7bar with GCI mode. Table 7 list the operating condition. Figure 28 shows corresponding simulation results of combustion pressure and HRR compared to engine test data. CFD has good agreement with engine data in capturing the fuel effects.

Table 7: Operating conditions for the fuel effect study at 1500rpm/IMEP$_{net}$ 7bar with GCI mode

Operating Conditions	
Engine Speed [rpm]	1500
IMEP$_{net}$ [bar]	7.0
Intake Pressure [kPa]	155
Intake Temperature [K]	326
Exhaust Pressure [kPa]	250
Exhaust Temperature [K]	598-600
CA50 [deg., aTDCf]	9
Fueling Injection	
Injection Pressure [bar]	300
SOI$_1$[deg., aTDCf]	-29.0
SOI$_2$ [deg., aTDCf]	-8.4 to -5.7
Split Ratio [-]	24/76

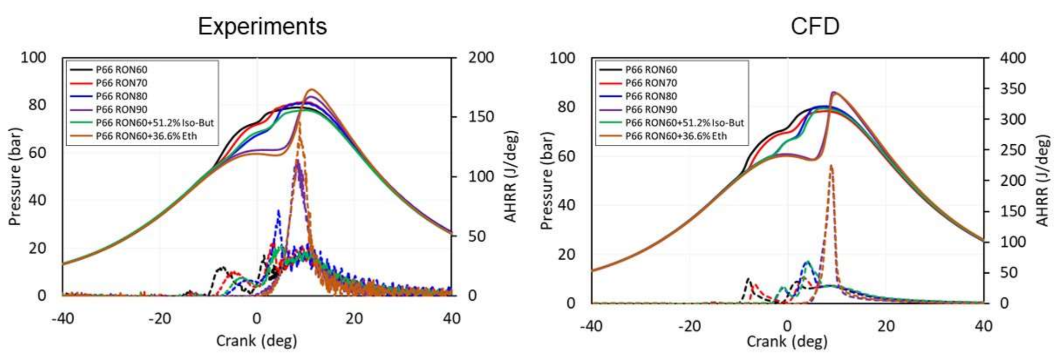

Figure 28: Combustion pressure and HRR for engine data and CFD simulations at 1500rpm/IMEP$_{net}$ 7bar with GCI mode.

3.6 Aftertreatment System Assessment

For this multimode lean gasoline engine, the LTC mode at low loads significantly reduces engine-out NOx and soot emissions, but leads to relatively higher CO and HC emissions as well as a low exhaust temperature that poses challenges for aftertreatment. Figure 29 shows an example of the engine-out emissions and exhaust temperature of load sweep at 2000rpm. In this case, LTC was used for BMEP up to 6bar, and GCI for higher load.

To meet ULEV70 and SULEV30 emissions standards, several different aftertreatment approaches were evaluated, and two aftertreatment system configurations were determined, as shown in Figure 30. The configuration A - SCR with Urea dosing - is estimated to be capable of meeting the ULEV70 emission standard. Adding a lean NOx trap (LNT) as in Configuration B will further reduce the tailpipe-out emissions to achieve SULEV30 emission standards.

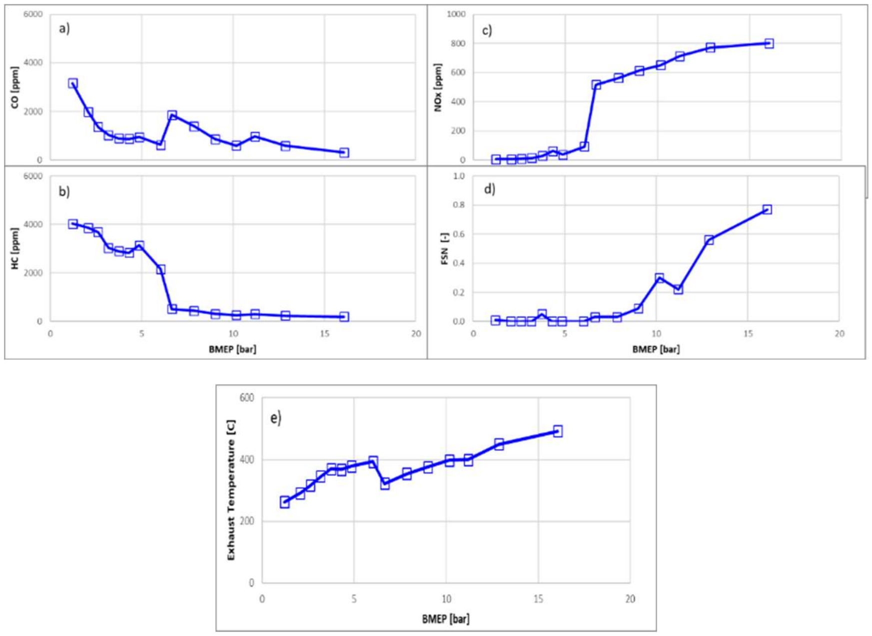

Figure 29: Emissions and exhaust temperature for load sweep at 2000rpm, with LTC for BMEP≤6bar and GCI for BMEP>6bar.

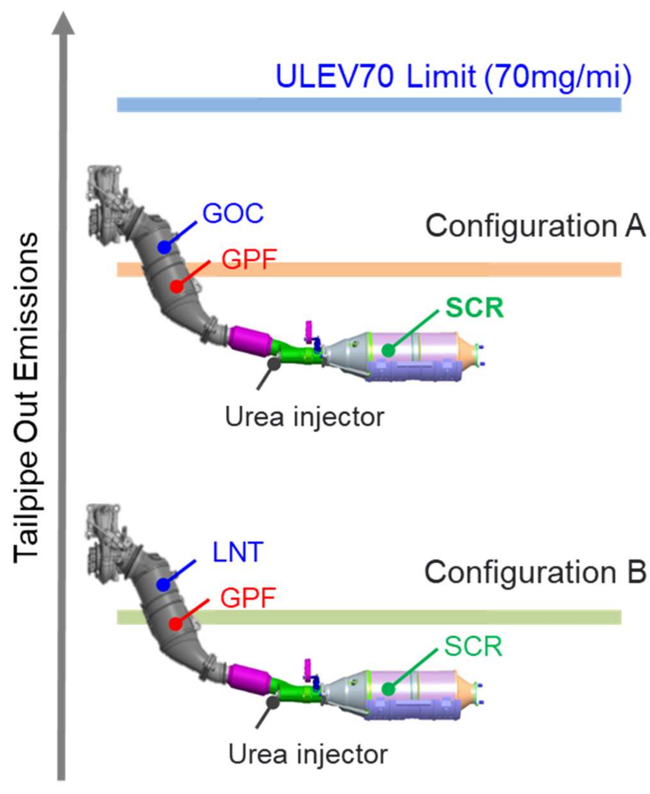

Figure 30: Aftertreatment systems for lean multimode GCI engine

For the CO and HC reductions at low temperature, the CuOx-CoOy-CeOz (CCC) catalysts tested in Oak Ridge National Laboratory [28] can be a good candidate. Figure 31 shows the corresponding CO and HC conversion efficiencies with 50:50 physical mixture of CCC with Pt/Al_2O_3. The 90% conversion of CO and HC was measured around 190^0C and 230^0C, respectively.

The engine-out soot emissions are very low for this multimode GCI engine, especially at low load with LTC mode. Packaging a small, catalyzed gasoline particulate filter (GPF) on the system would ensure ultra-low soot emissions during high load operation with a marginal penalty on fuel consumption.

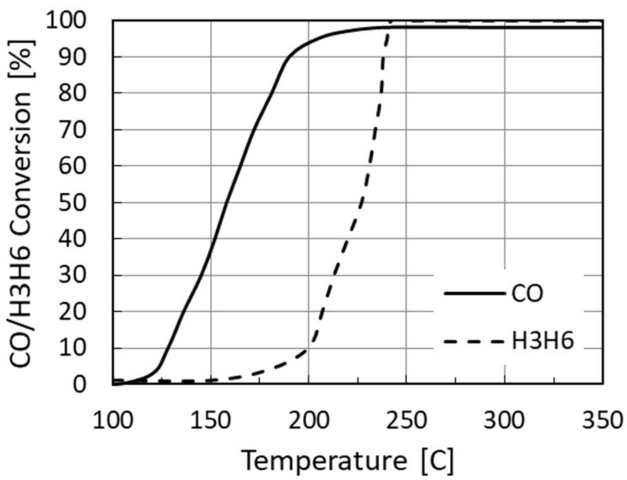

Figure 31: CO and HC light-off characteristics for 50:50 physical mixture of CCC with Pt/Al2O3 [28]

To reduce tailpipe-out NOx emissions, a close-coupled selective catalytic reduction (SCR) system is proposed. The urea injector is positioned upstream of the SCR catalyst. For the state-of-the-art control of NOx emissions from vehicles, NH_3-SCR with Cu-SSZ-13 zeolite component (Cu/Al=0.2, Cu=1.4 wt %) [29], the primary NOx reduction follows the "standard SCR" reaction of $4NO+4NH_3+O_2 \rightarrow 4N_2+6H_2O$ [nox-standard[30]. To further reduce NOx emissions at low temperature, it is necessary to use the "fast SCR" reaction using NO_2 as oxidant: $NO_2+2NH_3+NO_2 \rightarrow 2N_2+3H_2O$ [29]. Metal oxides such as cerium oxide (CeO_2) can catalyze NO oxidation to NO_2. Then coupling a metal –oxide-based selective catalytic oxidation phase and a zeolite-based SCR phase can facilitate selectively generating NO_2 in situ for faster SCR via bi-functional mechanism, and in turn, enhances low temperature activity in comparatively robust fashion. This dual-phase coupled catalyst also minimizes the dependency of SCR on NO_2 supply from the DOC [31]. Andana et al [29] shows for the combined Ceria-manganese oxide (CM) (Ce-to-Mn ratio=7:3) and Cu-SSZ-13 (CSZ) (Cu/Al=0.2, Cu=1.4 wt %) with 25wt% oxide to zeolite ratio, the NOx conversion efficiency is 50% at 205^0C and 90% at 264^0C, indicating good potential for low-temperature engines as this multimode GCI engine.

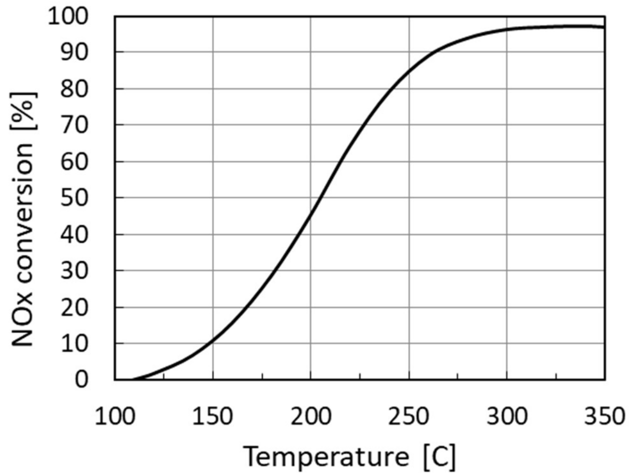

Figure 32: NOx light off characteristic for combined Ceria-manganese oxide (CM) (Ce-to-Mn ratio=7:3) and Cu-SSZ-13 (Cu/Al=0.2, Cu=1.4 wt %) with impregnation coupling technique for different oxide to zeolite ratio [29]

For the lean NO_x trap catalyst, the commercial LNT manufactured by Johnson-Matthey is proposed. The total precious metal loadings is 60 g/ft3 with the Pt/Rh ratio of 4:1. Li et al [32] shows the 90% NO_x conversion is located at 180-225^{0}C, depending on the redox history of the catalyst, as shown in Figure 33. With this additional LNT coupled before GOC, the tailpipe-out NO_x is expected to meet the SULEV30.

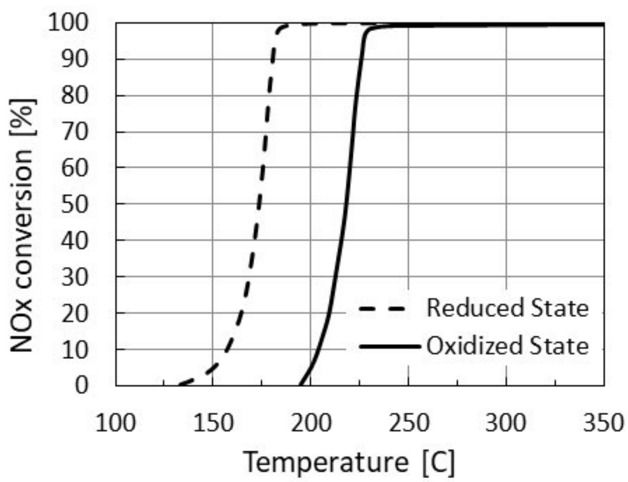

Figure 33: NOx light-off over reduced and oxided LNT [32]

3.7 FTP75 Drive Cycle

To evaluate the fuel economy (FE) improvement of the multimode combustion engine, an FTP75 drive cycle model was built with GT-SUITE by using engine test data. To better utilize the most efficient BTE island and also include some common state-of-the-art fuel economy applications, the gear shift schedule was optimized, start-stop feature was added, and engine downsizing and P2 full hybrid were also investigated.

Figure 34 a) and b) show the FTP75 residence plots over BTE map before and after gear shift schedule was optimized. Clearly, with the optimized gear shift, the high BTE points can be utilized. Figure 35 shows the progressive fuel consumption reduction for the 2.2L multimode GCI engine, GCI+biofuel iB25 (25% iso-butonal+75% RON60), downsized 1.5L GCI engine, and P2 hybrid. The multimode GCI engine can achieve 16% fuel economy improvement over the baseline SI engine, higher than the improvement target of 15%. By using iB25 biofuel, the FE improvement is increased to 18%. Downsizing the GCI engine to 1.5L results in about 30% fuel economy improvement over baseline SI engine. With the downsized engine and P2 full hybrid, the fuel economy can be then improved by 76%. Details of these improvements is shown in Figure 35.

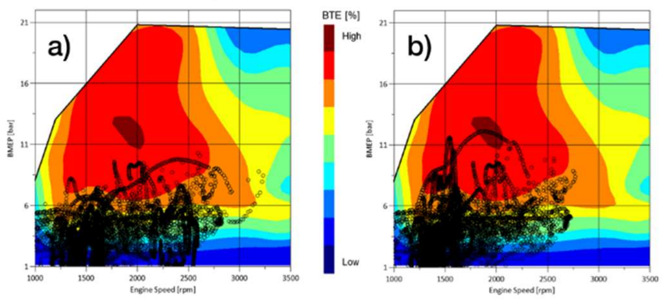

Figure 34: FTP75 residence plots over BTE contour for a) multimode GCI 2.2L engine, and b) gear optimization.

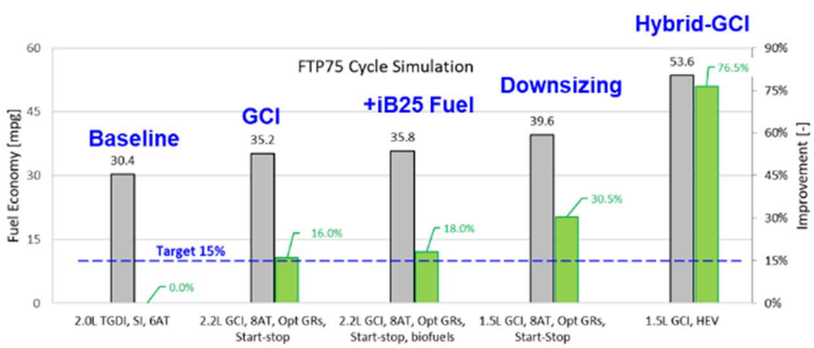

Figure 35: FTP75 Fuel consumption improvement

4 Summary and Conclusions

The multimode engine and control system including model-based combustion controllers and mode switching controller were designed. The proposed multimode GCI engine capable of SI, LTC and GCI was developed and tested. Combustion strategies were determined and successfully used to operate the engine in different modes and also switch combustion modes. It was demonstrated that this multimode GCI engine is feasible and capable of achieving a 16% improvement, or 18% with co-optimized fuel, in fuel economy compared to the production SI engine over a simulated FTP75 cycle while meeting ULEV70 standard. Additionally, a spray and combustion database with a high-pressure DI system with high-reactivity gasoline (60–90 RON) and biofuel blends under engine-like operating conditions was created, and used in the CFD spray model and the real fuel model can represent fuel physical properties and chemical kinetics of a real fuel. Then a physics-based CFD engine model was built and validated for multimode combustion simulations with different fuels.

5 Recommendations for Future Work

To meet the strict emission regulations of SULEV30 and EU7, confirming the aftertreatment system should be one of the focuses for future work. Investigating cold start emissions and developing reduction strategies would further help in addressing remaining emission concerns. Multimode engine control can be refined to improve the mode switching performance and test it under conditions that are more aggressive or extreme. Confirming engine performance at high speeds (>3500rpm) and high loads (>15bar BMEP) and also functionality and durability of high-pressure gasoline fuel system (e.g., 1800bar) would be essential to this multimode GCI engine concept. Additionally, utilizing the GCI operating points of high efficiency and low emissions for hybrid vehicle will be of interest and valuable.

6 Products Developed

<u>Publications</u>

- Zoldak, P.S., "Co-Optimized Fuel & Mixed-Mode GCI Engine-FY 19 Co-Optima" – Co-Optima Initiative-All Hands Meeting, Oakridge, March, 2019.
- Zoldak, P.S., "Co-optimized Fuel and Multi-Mode GCI Engine" Net Zero Technologies, SAE Innovations in Mobility Conference, Oct 31, 2019.
- Zoldak, P.S., "Co-optimized Mixed-Mode GCI Engine" –FY20 Co-Optima Initiative – All Hands Meeting Poster, Argonne National labs, March, 2020.
- Wagh, M., Joo, N.R., Zoldak, P.S., Won, H., Ra, Y., "Real Fuel Modeling for Gasoline Compression Ignition" SAE World Congress, 2020-01-0784.
- Zoldak, P.S., "Co-optimized Mixed-Mode Light-Duty Vehicle Engine" – VTO 2020 Annual Merit Review, Hyundai-Kia America Technical Center Inc. (HATCI), June, 2020.
- Zoldak, P.S., Naber, J.D., "Co-Optimized Multimode Light-Duty Engine (Hyundai America Technical Center Inc.), DOE VTO – Advanced Engine Technologies Annual Progress Report 2020, (i-22), 2021
- Zyada, A., Hollowell, J., Shirley, M., Fantin, N. et al., "Demonstration of Better than Diesel Efficiency and Soot Emissions using Gasoline Compression Ignition in a Light Duty Engine with a Fuel Pressure Limitation," SAE Technical Paper 2021-01-0518, 2021.
- Zoldak, P.S., and Zhu, S., "Hyundai Multi-Mode GCI Engine", Annual Merit Review, June 2021.
- Zhu, S., Naber, J.D., "Co-Optimized Multimode Light-Duty Engine (Hyundai America Technical Center Inc.)", DOE VTO – Advanced Engine Technologies Annual Progress Report 2021, (i-22), 2022
- Zhu, S., Shirley, M., Joo, N.R., Ha, K.P., Hollowell, J., Fantin, N., Revidat, S., Ullrich, J., "Technology Enablers for Advanced Gasoline Compression Ignition Engines", In: Kalghatgi G., Agarwal A.K., Goyal H., Houidi M.B. (eds) Gasoline Compression Ignition Technology. Energy, Environment, and Sustainability. Springer, Singapore, 2022. https://doi.org/10.1007/978-981-16-8735-8_2.
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<u>Thesis</u>

- Stanchina, Z., “An Experimental Study of Fuel Selection for a Gasoline Multimode, Spark Ignited – Compression Ignition Engine”, MS in Mechanical Engineering (August 2022).

Patents

- Zhu, S., Zoldak, P.S., Fantin, N., Zyada, A., Shirley, M., Hollowell, J., Ha, K.P.; “Multi-Mode Engine System and Associated Methods of Use,” disclosure has been accepted. July 2020.
- Zoldak, P.S., Zyada, A., Bourcier, M., Zhu, S., Joo, R.N., “Novel GDF (Gas Diffusion Flame) Combustion Mode and Hybrid Engine System,” disclose has been accepted. September 2020.
- Zhu, S., Hollowell, J., Shirley, M., Joo, N.R., Ha, K.P., Fantin, N., “Lean Burn Engine System and Associated Method of Use,” disclose has been accepted. September 2021.
- Shirley, M., Hollowell, J., Zhu, S., Joo, N.R., Ha, K.P., Fantin, N., “Split Cycle Waste Heat Method for Combustion Initiation in Gasoline Compression Ignition Engine,” disclose has been accepted. September 2021.

Other Products

- Spray and Combustion Data
- Fuel Surrogate Models and 3D CFD Engine Models

7 References

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8 Appendix I – Project Activity Summary

This project was conducted in three budget periods:

Budget Period 1: Engineering Research Design Phase

- Base “Mule” engine testing to establish baseline and zero dimensional (0D) boundary conditions. Hardware designs were completed, design reviews held, and hardware procurement kicked-off. Model build of baseline engine was completed. Fuel formulations were down-selected, and the identified bio-blends were characterized via spray and combustion studies along with merit function development.

Budget Period 2: Engineering Development Phase

- Engine controls development of cylinder pressure feedback controller was completed and coupled with exhaust gas recirculation (EGR) and boost controller. Mode switching and transient strategies were developed. Optical spray and combustion vessel (S&CV) testing and combustion simulation model refined with fuel formulation variants. Model validation for various fuel types was confirmed followed by engine and fuel co-optimization studies to define combustion recipe.

Budget Period 3: Engineering Validation Phase

- Further three dimensional (3D) computational fluid dynamics (CFD) modeling/analysis and design improvement to combustion recipe to ensure brake specific fuel consumption (BSFC), performance and emissions objectives are met. An engine was built and tested. Mixed-mode controls strategy was developed and optimization on a multi-cylinder test engine and one dimensional (1D) simulation was performed. Heat release analysis was performed and inputted into the 1D simulation vehicle modeling. Then it was followed by the validation of $\geq$15% fuel economy improvement target simulated on FTP-75.

The detail of activities and results from Budge Periods 1 can be found in [i,ii], and that for Budge Periods 2 in [iii,iv]. This final report mainly summarized the results from Budge Periods 3, since it includes the final demonstration and evaluation of the proposed multimode GCI engine in steady state operation, mode switching, and also the effect of co-optimized fuel formulation.

a. Original Hypotheses

- Originally the team had planned to go with Kefico 350 bar GDI and MPI fuel injectors. Recent developments on the Delphi Gen 3X GDCI program showed a solenoid actuated diesel like fuel injector with 1000bar capability is better suited for this program, in providing multiple and late injections at a higher rate and supporting gasoline diffusion flame which can help enabling higher engine loads and improving stability. It was decided to pursue GDI injector capable of 1000+ bar.
- Originally the team had planned to go with the mule engine of 2L Nu GDI 4-cylinder engine (CR 14). It was then changed to 2.2L R-TDI 4-cylinder (CR 16), for higher peak pressure and more favorable combustion chamber shape as well as a provision for a central DI injector.

b. Approaches Used

- 0D engine model – determining engine specifications for the performance targets.
- 1D engine simulation – matching boosting and EGR systems and investigating valve strategies to trap in-cylinder burnt gases, etc.
- 1D vehicle drive cycle simulation – determining fuel economy improvement, and studying common state-of-the-art fuel economy applications such as start-stop, downsizing, gear ratio optimization, and hybrid strategy.
- 3D CFD modeling – developing combustion strategies and optimizing combustion system.
- Fuel spray testing – to investigate the fuel effects and generate data for CFD model validation.
- Engine testing – validating engine control logics and algorithms, and developing combustion strategies, and demonstration of multimode combustion

c. Problems Encountered and Departure from Planned Methodology

1. Coolant leakage problem with GCI-01 engine.
2. State's executive order of state-at-home for limiting the spread of COVID-19 and COVID-19 protocols in place at HATCI.
3. Failures of two GCI-02 engines
4. COVID-19 restriction and labor shortage delayed the delivery of 1800bar gasoline fuel pump

d. Assessment of their impact on the Project Results

1. GCI-01 engine coolant leakage issue delayed engine testing and control validation. Some of control validation and refinement tasks were done with GCI-02 engine.
2. COVID-19 protocols limited engine testing time, but efforts on data analysis and engine modeling were increased to make best use of dyno time.

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[i] Zoldak, P.S., "Co-optimized Mixed-Mode Light-Duty Vehicle Engine," DOE VTO Annual Merit Review, June, 2020.
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3. The failures of two and only two GCI-02 engines necessitated engine rebuild and delayed the engine testing completion time. HATCI team made significant efforts to procure new parts and rebuild both engines, and together with MTU team were able to complete the needed engine tests within the program period.
4. 1000bar DI fuel system was used instead. For the rated condition where fuel pressure higher than 1000bar is needed, the validated CFD model was used to evaluate the combustion strategy and performance.