

Reactivity Controlled Compression Ignition Drive Cycle Emissions and Fuel Economy Estimations Using Vehicle Systems Simulations with E30 and ULSD

Scott Curran, Zhiming Gao, and Robert Wagner
Oak Ridge National Lab.

ABSTRACT

In-cylinder blending of gasoline and diesel to achieve reactivity controlled compression ignition (RCCI) has been shown to reduce NO_x and PM emissions while maintaining or improving brake thermal efficiency as compared to conventional diesel combustion (CDC). The RCCI concept has an advantage over many advanced combustion strategies in that the fuel reactivity can be tailored to the engine speed and load allowing stable low-temperature combustion to be extended over more of the light-duty drive cycle load range. However, the current range of the experimental RCCI engine map investigated here does not allow for RCCI operation over the entirety of some drive cycles and may require a multi-mode strategy where the engine switches from RCCI to CDC when speed and load fall outside of the RCCI range. The potential for RCCI to reduce drive cycle fuel economy and emissions is explored here by simulating the fuel economy and emissions for a multi-mode RCCI-enabled vehicle operating over a variety of U.S. drive cycles using experimental engine maps for multi-mode RCCI with E30 and ULSD, CDC and a variety of 2009 port-fuel injected (PFI) gasoline engines ranging from 1.8L to 4.0L. Simulations are completed assuming a conventional mid-size passenger vehicle with an automatic transmission that is optimized for each engine. RCCI fuel economy simulation results are compared to the same vehicle powered by a representative 2009 PFI gasoline engine over multiple drive cycles and showing at least a 20% improvement in fuel economy over a PFI baseline. Engine-out drive cycle emissions are compared to CDC and observations regarding relative gasoline and diesel tank sizes needed for the various drive cycles are also summarized.

CITATION: Curran, S., Gao, Z., and Wagner, R., "Reactivity Controlled Compression Ignition Drive Cycle Emissions and Fuel Economy Estimations Using Vehicle Systems Simulations with E30 and ULSD," *SAE Int. J. Engines* 7(2):2014, doi:10.4271/2014-01-1324.

INTRODUCTION

The United States Department of Energy (DOE), Vehicle Technologies Office's (VTO) mission is to develop more energy-efficient and environmentally friendly highway transportation technologies that will enable the United States to use significantly less petroleum and reduce greenhouse gas emissions and criteria air pollutants [1]. Fuel efficiency improvements and petroleum displacement are the overarching goals of the DOE VTO and within these research activities, resolving the interdependent emissions challenges from high efficiency engines is important. Emissions challenges are relevant not only in terms of market barrier and regulatory standpoints, but also in terms of total engine system fuel efficiency. Engine system efficiency includes not only the fuel energy required for the production of motive or shaft power, but also the fuel penalties associated with exhaust aftertreatments and sub-optimal combustion (i.e. stoichiometric spark ignition allowing a three-way catalyst or retarded injection timing for NO_x control in compression ignition engines). For diesel engines operating lean, these fuel penalties include fuel

regeneration of diesel particulate filters (DPF) and either fuel regeneration of lean NO_x traps (LNT), or reductant addition for selective catalytic reduction (SCR) systems. Within the DOE VTO, the Advanced Combustion Engine research and development subprogram's strategic goals are to reduce petroleum dependence by removing critical technical barriers to mass commercialization of high-efficiency, emissions-compliant internal combustion engine powertrains in passenger and commercial vehicles [2]. Improvements in engine efficiency and engine systems efficiency through advanced combustion strategies is an important pathway to this goal. For advanced combustion strategies to be able to meet these goals, their effectiveness over driving cycles [3] will have to be determined.

In the United States, the U.S. Environmental Protection Agency (EPA) regulates emissions based on federal drive cycle compliance [3]. There are a number of EPA dynamometer driving cycles which attempt to take into account the real world driving conditions seen with light-duty passenger vehicles. If a the engine cannot be operated in an advanced combustion mode over the entire speed and load range demanded by all

the regulatory drive-cycles, then the engine would have to operate in a multi-mode strategy in which the engine would switch to a conventional combustion mode when engine power demands cause the engine to operate outside of the advanced combustion speed and load operating range. The need for multi-mode operation has implications for the design of the fuel system and combustion geometry to allow this as well as the aftertreatment system which will need to allow for emissions compliance over both modes.

In-cylinder blending of gasoline and diesel to achieve reactivity controlled compression ignition (RCCI) has been shown to reduce NO_x and PM emissions while maintaining or improving brake thermal efficiency as compared to conventional diesel combustion (CDC). The ability to control the percent premixed low reactivity fuel along with the timing and number of injections of the direct injected high reactivity fuel reactivity allows for not only reactivity stratification but also temperature and equivalence ratio stratification in the cylinder providing further control of combustion phasing and cylinder pressure rise rate. The RCCI concept as shown in [figure 1](#), has an advantage over many advanced combustion strategies [[4](#), [5](#), [6](#), [7](#), [8](#), [9](#), [10](#), [11](#)] in that the fuel reactivity can be tailored to the engine speed and load allowing stable low-temperature combustion to be extended over more of the light-duty drive cycle load range [[12](#)] and allow for increased controllability over the combustion process.

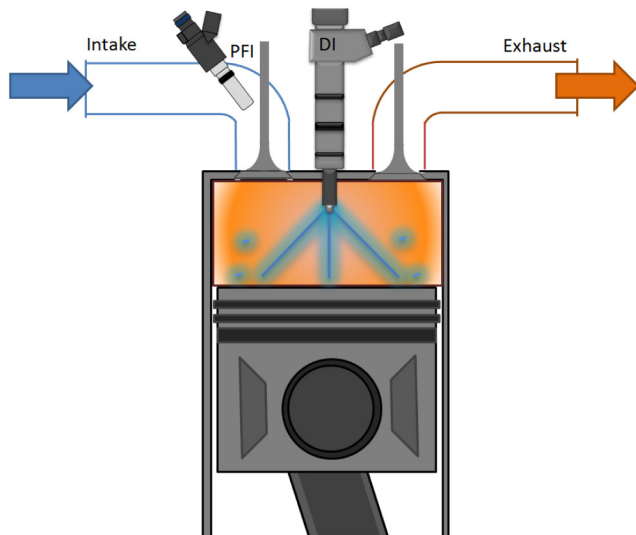


Figure 1. Dual-Fuel RCCI Injection Strategy

Previous computational fluid dynamics (CFD) modeling and single cylinder engine (SCE) results have demonstrated high gross thermal efficiencies (GTE) with ultra-low NO_x and soot emissions with RCCI. Thorough reviews of RCCI SCE experiments and CFD modeling advances can be found in papers by Kokjohn, Splitter, Hanson and Reitz [[12](#), [13](#), [14](#), [15](#), [16](#)].

Previous experiments have investigated the translational effects of taking CFD modeling and single cylinder engine experiments to multi-cylinder engines (MCE) on efficiency, emissions, and controls [[17](#), [18](#), [19](#), [20](#), [21](#), [22](#), [23](#)]. These

effects include the behavior of real turbomachinery, effects of real EGR, cylinder to cylinder imbalances and swirl with production viable engine components. Despite the translational effects, MCE RCCI has been shown to be capable of diesel-like efficiency at lower engine loads and greater than diesel efficiency at higher engine loads with an order of magnitude reduction in engine out NO_x as compared to CDC. Previous experiments have shown the benefits of increased control over the combustion process allowed by RCCI operation on extending the operating range of low temperature combustion (LTC) compared to diesel premixed charge compression ignition (PCCI) on a multi-cylinder light-duty compression ignition engine [[19](#), [20](#)].

There have been a number of studies examining the potential for multi-mode LTC/CDC operation with diesel engine baselines for PCCI and more recently RCCI [[24](#), [25](#)]. For LTC/CDC multi-mode operation, the engine switches to CDC for areas of the engine map that fell outside LTC region. The need for multi-mode operation has implications for the needs of the aftertreatment system to be able to meet stringent federal emissions standards over the prescribed drive cycles, namely for NO_x control if the engine has to switch to CDC mode for higher loads in regions of the map that produce high amounts of NO_x .

It is difficult to draw conclusions on light-duty drive cycle fuel economy and emissions performance for combustion strategies in the development stage which only have demonstrated a limited number of steady state operating points. To date there have been few published studies that investigate the potential vehicle fuel economy improvements that RCCI could allow. Previous studies by Curran et al. [[19](#), [20](#)] looked at using the Fuels Working group's ad-hoc modal points [[7](#)] to estimate drive cycle emissions with RCCI as compared to conventional diesel combustion. These modal points are representative of key areas of the federal drive testing protocol and have weighting factors attached to them linked to the amount of drive cycle spent at similar conditions. That work showed that the ability to obtain noise constrained RCCI operation over all of the ad-hoc modal points was dependent on the fuels used. The light-duty MCE experiments showed that the hard acceleration modal point of 2600 RPM, 8.8 bar BMEP was not obtainable with a 46 Cetane ULSD and certification gasoline with an RON of 96 (UTG-96) [[20](#)] while adhering to a cylinder pressure rise rate limit of 10bar/deg. A follow-up study showed that the 2600 RPM, 8.8 bar BMEP point was achievable with RCCI using E85 and ULSD [[19](#)]. The results of the RCCI modal point studies showed significant weighted composite NO_x reductions (~66%) were made possible with RCCI operation as compared to CDC. The results also showed significant increases in engine out HC and CO emissions resulted from RCCI operation. The RCCI modal point studies only examined estimated drive cycle emissions and did not attempt to apply the weighting factors to fuel economy improvements.

Vehicle systems simulation tools such as Autonomie developed by Argonne National Laboratory for the Department of Energy can be used to simulate vehicle operation using model based simulations [26]. The simulations use performance based measurements including fuel consumption and exhaust properties such as emissions and temperature which are tabulated allowing for the generation interpolated response surfaces over the entire operating range of the engine maps. Previous work by Gao et al. has demonstrated the use of steady state engine maps in transient drive cycle simulations [27, 28]. Previous work by Gao has examined this type of simulation with multi-mode advanced combustion steady state engine data for engine performance and emissions modeling [28].

Initial drive cycle performance modeling using vehicle systems simulations using engine maps [29] derived from experimental data in Curran and Gao [showed multi-mode operation RCCI/ CDC had the potential to offer greater than 15% fuel economy improvement over representative 2009 gasoline PFI baselines over many light-duty driving cycles [30]. RCCI fuel economy improvements were observed despite lack of complete drive cycle coverage. These simulations were performed on the same engine being investigated in this study using certification grade gasoline and B20 (20% biodiesel, 80% diesel) for the DI fuel. The results showed how much of an effect multi-mode operation can have on engine out NO_x emissions depending on the amount of the drive cycle coverage that RCCI operation can allow. Modeled drive cycle emissions results showed between a 17% and 21% reduction in NO_x with multi-mode RCCI as compared to diesel only operation. If an engine has to switch to CDC operation during high engine loads, the engine out NO_x will be very high and quickly can degrade the NO_x reduction potential of RCCI. Fuel usage over the drive cycles showed that nearly equal amounts of gasoline and diesel fuel would most likely needed to be carried on board for RCCI multi-mode operation. During RCCI only operation fuel usage was found to be between 57% and 69% gasoline.

The ability of ethanol fuels to increase the high load operating range of RCCI with potential compromise to the lower load operability and the effect on drive cycle coverage is not well understood. This work investigates the potential fuel economy of multi-mode RCCI operation using vehicle systems simulations with experimental steady-state engine maps compared to a representative 2009 gasoline PFI engine as baseline for comparison using diesel fuel and E30 (30% ethanol, 70% gasoline). Experimental steady-state RCCI operating points on modified multi-cylinder GM 1.9-L engine using an in-house methodology for RCCI combustion were used to develop an RCCI speed/load map consistent with a light-duty drive-cycle with sufficient detail to support vehicle simulations. The RCCI map developed as part of this study represents an increase in RCCI operation over previous low temperature combustion operation maps [30], but was still not able to cover the engine speed and load required to meet all power demands over the light-duty drive cycles with the self-imposed constraints imposed on the engine experiments

leading to the RCCI engine map. The simulations used a multimode RCCI/diesel operating strategy where the engine would operate in RCCI mode whenever possible but at the highest and lowest engine operating points, the engine would switch to diesel mode. All simulations were carried out in Autonomie using a 1580 kg passenger vehicle (mid-size sedan i.e. Chevrolet Malibu) over numerous U.S. federal light-duty drive cycles. A representative 2009 gasoline PFI engine map was obtained from an automotive original equipment manufacturer (OEM) for use in the vehicle simulations. A 2009 gasoline PFI baseline is standard in DOE VTO programmatic goals [1,2]. RCCI fuel economy simulation results are compared to the same vehicle powered by a representative 2009 PFI gasoline engine over multiple drive cycles Engine-out drive cycle emissions are compared to CDC and observations regarding relative gasoline and diesel tank sizes needed for the various drive cycles are also summarized.

METHODOLOGY

For this study 6 engine maps were used for the vehicle systems simulations. A multi-mode experimental RCCI map, which is described in the next section, was used along with a CDC map for multi-mode operation. An experimental CDC map was used using the stock pistons with the same base engine used for the RCCI experiments. CDC mapping was conducted on the base engine with the OEM pistons using Euro IV calibrations maps providing fuel consumption and emissions data for the simulations. Experimental naturally aspirated 2009 PFI gasoline engine maps ranging 1.8L to 4.0L were provided by an OEM partner. The PFI maps were for fuel consumption only so no comparisons with modeled emissions can be made. The fuel economy modeling was performed with using vehicle systems simulations with experimental engine data.

Experimental RCCI Mapping

Experimental Setup

The engine used for this study is a modified 2007 General Motors 4 cylinder 1.9L turbocharged diesel engine. The base engine has a rated power of 110 kW and a rated torque of 315 Nm. The original equipment manufacturer (OEM) pistons were replaced with pistons modified for RCCI. The RCCI modified piston bowl geometry was designed for RCCI using CFD modeling by UW. The piston design is based on a heavy duty piston and minimizes the surface area of the piston to minimize heat transfer losses and also results in a lowered compression from 17.1 in the OEM configuration to 15.1 to allow for higher load operation while maintaining reasonable pressure rise rate limits. More information about the piston design can be found in the paper by Hanson et al [23]. The diesel injection system and variable geometry turbo charger (VGT) were left in production form. The intake manifold was modified to incorporate extended tip narrow spray angle PFI injectors for the gasoline supply. A more in-depth discussion the intake manifold modifications can be found in Curran et al [20]. Figure 1 shows the overall fuel system layout for RCCI operation.

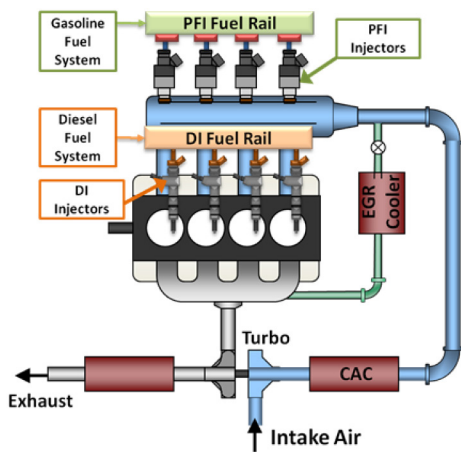


Figure 2. ORNL Multi-Cylinder RCCI Engine

Table 1 shows engine specifications for the base engine.

Tables 2 and 3 show the injector specifications for the DI and PFI injectors respectively.

Table 1. GM 1.9 L CIDI Base Configuration

Number of Cylinders	4
Bore (mm)	82.0
Stroke (mm)	90.4
Compression Ratio	15.1

Table 2. Diesel injector specifications

Number of Nozzle Holes	7
Included Spray Angle (°)	148

Table 3. Port-fuel injector specifications

Number of Nozzle Holes	4
Cone Angle (°)	15
Separation Angle (°)	22

The stock ECU was replaced with a full-pass DRIVEN control system which allowed simultaneous control of the PFI and DI fuel systems and all other engine parameters. Engine torque was measured using an absorbing eddy-current dynamometer. The DI fuel flowrate was measured with a Micro Motion Coriolis fuel meter, while the PFI fuel flowrate was measured using a Max Machinery 710-213 positive displacement volumetric flow measurement system. The intake air flowrate was measured using a laminar flow element and the stock intake mass-airflow sensor.

Engine-out emissions were measured using standard analysis techniques. A heated flame ionization detector (FID) was used to measure total unburned hydrocarbons. A heated chemiluminescence (CLD) instrument was used to measure NO_x . CO and CO_2 were measured using non-dispersive infrared (NDIR) instruments. Intake and exhaust O_2 was measured using a paramagnetic detector (PMD). Both intake

and exhaust CO_2 were measured to provide the EGR rate. Sampled gas streams were chilled to remove water prior to measurement by PMD and NDIR instruments. Both intake and exhaust sample streams were conveyed from heated filters to the instruments through heated lines maintained at 190°C . Conditioned air was supplied to the engine at a constant temperature of 25°C and a relative humidity of 58%. An AVL 415S smoke meter was used to measure filter smoke number (FSN). A limitation to using a smoke meter based on the blackening of filter paper (reflectivity) is that it may not accurately account for condensable organic hydrocarbons in the PM, which have been shown to be the primary PM mode with RCCI. Previous studies have compared the results of FSN and PM filter mass measurements from RCCI operation and have shown that the RCCI PM is mostly organic carbon with almost no elemental carbon [29, 30]. Engine emissions as well as important temperatures, pressures, flowrates as well as engine speed and torque were sampled for 180 seconds after 120 seconds of stable operation had been attained.

High speed combustion data was acquired using Kistler model 6058A pressure sensors installed in the glow plug ports of all 4 cylinders. Individual Kistler type 5010 Dual-Mode Amplifiers were used to process the pressure signals and the built in combustion package from Driven was used to process the data. Combustion metrics were monitored and recorded using the DRIVEN combustion analysis toolkit (DCAT). All brake thermal efficiencies presented here are calculated using the lower heating value (LHV) of the fuels used and brake power as measured from the dynamometer.

Table 4. Fuel specification for E30 and ULSD

Specification	E30	ULSD
Lower Heating Value (kJ/kg)	37742	42880
Specific Gravity	0.7445	0.848
H (weight %)	13.73	13.2
C (weight %)	74.4	86.8
Oxygen (weight %)	11.34	0
Aromatics (weight %)	16.4	29.9
Ethanol (vol %)	32.59	0
Initial Boiling Point ($^\circ\text{C}$)	86	184
Final Boiling Point ($^\circ\text{C}$)	379	332
Research Octane Number (RON)	101.3	NA
Motor Octane Number (MON)	88.5	NA
(RON + MON)/2	94.9	NA
Cetane Number	NA	42.5

The DI fuel used in this study was a 2007 certification grade Ultra Low Sulfur Diesel (ULSD) fuel with a cetane number of 42.5, the PFI fuel was an E30 gasoline/ethanol blend with an anti-knock index (AKI) of 92.1 The E30 was splash blended with 30% anhydrous ethanol and 70% 87 AKI gasoline containing no ethanol. Ethanol blends had been previously shown to allow for improvements in the high load RCCI