In-cylinder blending of gasoline and diesel fuels to achieve low-temperature reactivity controlled compression ignition (RCCI) can reduce NOx and PM emissions while maintaining or improving brake thermal efficiency compared to conventional diesel combustion (CDC). Moreover, dual-fueling is able to achieve these benefits by tailoring combustion reactivity over a wider range of engine operation than is possible with a single fuel. However, the currently demonstrated range of stable RCCI combustion just covers a portion of the engine speed-load range required in several light-duty drive cycles. This means that engines must switch from RCCI to CDC when speed and load fall outside of the stable RCCI range. In this study we investigated the potential impact of RCCI on the engine-out exhaust temperature and emissions of a multi-mode RCCI-enabled vehicle operating over two urban and two highway driving cycles. To implement our simulations, we employed experimental RCCI/CDC engine maps combined with a standard mid-size, automatic transmission, passenger vehicle configuration details in the Autonomie vehicle simulation platform. Our results include both detailed transient and cycle-averaged engine exhaust temperature and emissions. We note the potential implications of the modified exhaust properties on catalytic emissions control and utilization of waste heat recovery on future RCCI-enabled vehicles.

1. Introduction

Typically, RCCI combustion involves introduction of a low reactivity fuel into the cylinder to create a pre-mixed initial charge, followed by direct injection of a higher reactivity fuel before ignition of the premixed fuel occurs [1]. This is usually referred to as dual-fuel RCCI. The dual-fuel RCCI strategy considered in this paper is the combination of PFI gasoline and DI diesel, as is illustrated in Figure 1. By introducing gasoline and diesel at different locations and timing in the cycle, it is possible to stratify equivalence ratio, reactivity, and temperature inside the cylinder prior to and during combustion. Thus both combustion phasing and cylinder pressure rise rate can be controlled to increase brake thermal efficiency while lowering NOx and particulates [2-6]. An advantage of RCCI over other advanced combustion strategies is the high flexible in combustion management [7–14]. That is, by modulating the amount of each fuel and the timing of the high reactivity fuel, global fuel reactivity as well as the reactivity stratification can be varied with engine speed and load, allowing low-temperature combustion to be stabilized over a wider drive cycle range [2]. Even in the more complex conditions of multi-cylinder engines, the reported experiments have demonstrated that RCCI produces diesel-like brake
thermal efficiency at low loads and greater than diesel brake thermal efficiency at high loads with an order of magnitude reduction in engine out NOx as compared to CDC [15-21]. Moreover it is possible to extend 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 [17, 18].

One potential barrier to widespread RCCI utilization is that, at higher speeds and loads, the pressure rise rate can become sufficiently high to damage the engine. Thus it is necessary to constrain RCCI operation to regions of the full engine speed and load range where the pressure rise rate is below a critical value. In cases where the drive cycle demands require engine operation outside the RCCI-accessible limits, it is necessary to switch the combustion mode to CDC. Likewise, when the speed and load demands return to the RCCI-accessible region, it is possible to switch back to RCCI. A key concern of the present study is to understand how this bi-modal operation could affect the engine exhaust characteristics for different drive cycles.

Previous studies by Curran et al. [17, 18] utilized ad-hoc steady-state dynamometer modal points [10] to estimate drive cycle emissions with RCCI as compared to conventional diesel combustion. There have also been other studies examining the potential for LTC/CDC multi-mode operation with diesel engine baselines [22, 23]. The challenge is to estimate fuel economy and emissions performance for realistic drive cycles when the advanced combustion strategies of interest have only been demonstrated for a limited number of steady-state operating points. Vehicle systems simulation tools such as Autonomie (developed by Argonne National Laboratory for the Department of Energy) can be used to simulate drive cycles if adequate engine models are available [24]. Typically, Autonomie simulations utilize steady-state maps for fuel consumption and engine-out exhaust properties that have been tabulated from experimental measurements. Recently, studies at ORNL have demonstrated that it is possible to also simulate the impact of drive cycle transients on engine performance, thus accounting for important effects not normally included in steady-state simulations [25, 26]. This transient simulation approach has previously been applied to other types of multi-mode advanced combustion [26].

In this work we investigated the potential engine-out emissions from multi-mode RCCI operation under multiple light-duty drive cycle conditions. We estimated the engine-out exhaust properties from computational simulations of a light-duty vehicle with an engine model based on experimental steady-state maps combined with a previously published methodology to account for drive cycle transients [25]. The maps were constructed from dynamometer measurements of a modified light-duty multi-cylinder diesel engine operating in both CDC and RCCI modes. The RCCI operating points in this map represent an increase in RCCI operating range compared to previous low temperature combustion maps [27], but it did still not cover the entire speed and load requirements of the simulated light-duty drive cycles. Thus we used a multi-mode RCCI/diesel operating strategy in which the engine would operate in RCCI mode whenever possible but at the highest and lowest engine operating points, the engine would switch to CDC. All simulations were carried out in Autonomie using a 1580 kg passenger vehicle (mid-size sedan i.e. Chevrolet Malibu) over several light-duty drive cycles. Engine-out drive cycle emissions for both CDC only and CDC/RCCI operation are compared.

2. Experimental

The simulated engine in this study was a modified 2007 General Motors 4-cylinder, 1.9L turbocharged diesel. The base engine has a rated power of 110 kW and a rated torque of 315 Nm. For RCCI operation, the original manufacturer pistons were replaced with open bowl pistons which have a lower surface area and lowering the compression ratio from 17.1 to 15.1. More information about the piston design can be found in the paper by Hanson et al [21]. The diesel injection system and variable geometry turbo charger (VGT) were left unchanged. The intake manifold was modified to incorporate extended tip narrow spray angle port fuel injectors (PFIs) for the gasoline supply. A more in-depth discussion the intake manifold modifications can be found in Curran et al [18]. Figure 2 shows the overall fuel system and engine layout. Table 1 summarizes the modified engine specifications, and summarizes the key specifications for the direct injection (DI) and PFI injectors respectively.
Figure 2. Schematic representation of the ORNL multi-cylinder 1.9L RCCI-capable engine used to generate the engine-out data for this study.

Table 1. GM 1.9 L CIDI engine Base Configuration and specifications of diesel and port-fuel injector

<table>
<thead>
<tr>
<th>CIDI Base Configuration</th>
<th>Number of Cylinders</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Bore (mm)</td>
<td>82.0</td>
</tr>
<tr>
<td></td>
<td>Stroke (mm)</td>
<td>90.4</td>
</tr>
<tr>
<td></td>
<td>Compression Ratio</td>
<td>15.1</td>
</tr>
<tr>
<td>DI specifications</td>
<td>Number of Nozzle Holes</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>Included Spray Angle (°)</td>
<td>148</td>
</tr>
<tr>
<td>PFI specifications</td>
<td>Number of Nozzle Holes</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>Cone Angle (°)</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Separation Angle (°)</td>
<td>22</td>
</tr>
</tbody>
</table>

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

Engine exhaust temperature was measured with a standard K-type thermal couple. A heated flame ionization detector (FID) measured total unburned HCs, and NOx was measured with a chemi-luminescence (CLD) detector. CO and CO₂ were measured with non-dispersive infrared (NDIR) instruments. Intake and exhaust O₂ was measured by a paramagnetic detector (PMD). Both intake and exhaust CO₂ were measured to provide the EGR rate. Sampled gases were chilled prior to being routed to the 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) [27, 28].

Engine emissions as well as temperatures, pressures, flows, speed, and torque were sampled for 180 seconds after 120 seconds of stable operation had been attained. High speed cylinder pressures in all 4 cylinders were measured with Kistler model 6058A sensors installed in the glow plug ports. Individual Kistler type 5010 Dual-Mode Amplifiers were used to process the pressure signals and the built in combustion package from Drivven was used to process the data. Combustion metrics were monitored and recorded using the DRIVVEN combustion analysis toolkit (DCAT). The DI fuel used in this study was a B20 biodiesel blend consisting of 20% biodiesel and 80% 2007 certification grade Ultra Low Sulfur Diesel (ULSD) fuel with a cetane number of 42.5. Adding 20% biodiesel had been shown to improve both low- and high-load RCCI performance as compared to the ULSD diesel fuel [20]. The PFI gasoline fuel was UTG 96 with an anti-knock index (AKI) of 92.1 containing no ethanol.
Steady-state engine exhaust measurement points were designed to systematically cover speed and load ranges previously established for CDC and RCCI operation of the GM engine [18]. Figure 3 depicts the boundaries of CDC operating envelope with the RCCI operating region superimposed. Colors indicate differences in brake thermal efficiency (BTE) associated with using RCCI. Grid points mark the locations where measurements were made to construct the steady-state emissions and temperature maps. Similar maps were constructed for the steady-state exhaust temperature and emissions, including NOx, HCs, CO, and PM from the collected measurements using standard surface fitting algorithms in Matlab. The large impact of RCCI on steady-state engine-out emissions is depicted in Figure 4 where the NOx and HC levels in the RCCI domain are depicted.

![Figure 3. Depiction of the operating boundaries for CDC and RCCI operation of the GM 1.9L experimental engine. Green grid points indicate experimental RCCI locations. Colors indicate where RCCI BTE is higher than for CDC.](image)

3. Simulation Methodology

Vehicle drive cycle simulations were performed using the Autonomie vehicle simulation platform [29]. For the vehicle configuration, we selected the default Autonomie parameters for a conventional 1,580kg mid-size passenger car with an automatic transmission. The steady-state experimental engine maps described above were combined with a previously published methodology to account for engine transients under drive cycle conditions [25]. The details of this methodology are beyond the scope of present discussion, but in brief, the simulated exhaust temperature and composition were adjusted from their nominal steady-state values by applying dynamic first-order correction factors and a small number of empirical parameters that account for the inherent thermal and combustion lags in the engine as it shifts from one state to another. As explained in [25], previous studies have shown that resulting simulated transient exhaust properties agree well with experimental chassis dynamometer measurements for similar light-duty engines.
Our drive cycle simulations included comparisons between a vehicle operating in CDC-only and a vehicle with an engine capable of multi-mode RCCI/CDC. While it was possible to utilize RCCI to some extent in all the simulated drive cycles, in all cases there were periods when engine conditions moved out of the RCCI operating range, and the engine had to shift back to CDC. When such transients were required, we assumed a perfect step change in combustion, which is clearly a limitation of the present study that should be addressed in the future.

To better understand the impact of RCCI might affect engine-out emissions from a conventional passenger car, we simulated four city and highway driving cycles: the Urban Dynamometer Driving Schedule (UDDS), the Highway Fuel Economy Driving Schedule (HWFET), the US06 cycle, and the New York City driving cycle (NYCDC) (see Figure 5). Details of these cycles can be found at [30]. The UDDS and New York cycles represent urban driving with frequent stopping. The HWFET represents highway driving under 60 miles per hour, and the US06 cycle includes aggressive accelerations and decelerations combined with highway driving. All of the above cycles were assumed to start with a fully warmed engine, and thus no cold start effects were considered in the present study. This is clearly another limitation of the present study that needs to be expanded in the future.

Figure 5. Speed profiles for the four driving cycles included in this study.

4. Results and Discussion

Figure 6 shows how the RCCI domain overlaps with the speed-load demands for each of the different simulated drive cycles. Each point indicates the engine speed and load at 1 second intervals throughout the drive cycle. Colors indicate the engine BTE. Clearly the accessibility of RCCI is highly dependent on the specific drive cycle given the current speed and load restrictions associated with RCCI operation. Table 2 summarizes the fraction of each drive cycle during which RCCI was available. On a distance travelled basis, RCCI could cover 72% of the UDDS cycle but only 55% of the UDDS cycle time, since there were significant periods of very low load and idling. In the HWFET RCCI could be utilized over 88% of the distance and 86% of the time. The simulated cumulative engine-out emissions for each drive cycle with RCCI enabled are summarized in Table 3 relative to the corresponding levels for CDC-only operation.
Figure 6. RCCI utilization during each drive cycle. Blue points mark instantaneous speed and load at 1 s intervals.

Table 2. Multi-mode RCCI utilization for each simulated drive cycle.

<table>
<thead>
<tr>
<th>RCCI results</th>
<th>% drive cycle by Distance</th>
<th>% drive cycle by time</th>
<th>Total diesel fuel</th>
<th>% Diesel during RCCI</th>
</tr>
</thead>
<tbody>
<tr>
<td>UDDS</td>
<td>72%</td>
<td>55%</td>
<td>56%</td>
<td>41%</td>
</tr>
<tr>
<td>HWFET</td>
<td>88%</td>
<td>86%</td>
<td>44%</td>
<td>37%</td>
</tr>
<tr>
<td>US06</td>
<td>66%</td>
<td>56%</td>
<td>66%</td>
<td>31%</td>
</tr>
<tr>
<td>NYCC</td>
<td>69%</td>
<td>36%</td>
<td>65%</td>
<td>43%</td>
</tr>
</tbody>
</table>

Table 3. Simulated change in cumulative emissions between dual-mode (CDC/RCCI) operation and CDC-only operation (plus sign in red indicates an increase).

<table>
<thead>
<tr>
<th>Reductions With RCCI</th>
<th>PM</th>
<th>NOx</th>
<th>HC</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>UDDS</td>
<td>-56%</td>
<td>-3%</td>
<td>+242%</td>
<td>+154%</td>
</tr>
<tr>
<td>HWFET</td>
<td>-68%</td>
<td>-21%</td>
<td>+302%</td>
<td>+140%</td>
</tr>
<tr>
<td>US06</td>
<td>-33%</td>
<td>-8%</td>
<td>+312%</td>
<td>+137%</td>
</tr>
<tr>
<td>NY City</td>
<td>-62%</td>
<td>+4%</td>
<td>+219%</td>
<td>+152%</td>
</tr>
</tbody>
</table>
The PM reductions associated with RCCI (as measured by filter smoke number) in all of the city and highway driving cycles were very significant, as the PM reduction over the UDDS and HWFET were between 56 and 68% as compared to CDC operation. However, the reductions in UDDS and HWFET NOx associated with RCCI were just between 3 and 21% as compared to CDC operation. The effect of RCCI on NOx reduction was also limited in the other two cycles. It appears that the most beneficial effects of RCCI occur when it helps avoid the high NOx excursions from CDC during higher load operation. Clearly the present limitation on RCCI utilization during realistic drive cycles significantly reduces its potential NOx benefit. This is discussed later in details. In addition, the large increases in HCs and CO imply that robust catalytic oxidation aftertreatment will still be needed for meeting emissions regulations.

More detailed comparisons of the transient engine-out emissions for CDC/RCCI and CDC-only operation are depicted in Figure 7 for the UDDS cycle. As noted above, it appears that the biggest NOx benefit from RCCI occurs when the high NOx excursions associated with high load operation can be reduced. This suggests that extending the accessible high load domain of RCCI should be one of the highest priorities in advancing the state of the art.

Besides emissions, RCCI significantly affects exhaust temperature, since higher BTE typically means that less fuel energy is passed on to the exhaust. This is important because lower exhaust temperatures can pose a significant challenge for catalytic aftertreatment and potential use of recovered waste heat. Figure 8 depicts the simulated transient exhaust temperatures from this study for both the CDC/RCCI and CDC-only modes during the UDDS cycle. As expected, utilization of RCCI significantly reduced exhaust temperatures. The largest temperature reductions appeared during temperature spikes, but there were also differences of approximately 10°C in the temperature minima. Given the much higher levels of HC and CO when RCCI is used, such low temperatures could pose significant problems for HC and CO emissions control.
As discussed above, the reductions in NOx associated with RCCI were limited as compared to CDC operation. Figure 4 reveals that significant NOx reductions could be achieved with RCCI, if it can be used during higher load operation instead of CDC. To simulate this scenario, we altered the vehicle transmission controls so that the engine is able to avoid the high speed-load range above the RCCI limit during the UDDS cycle. The simulated UDDS results are illustrated in Figure 9.

These results imply that with the altered transmission controls, RCCI could improve fuel economy by about 5% as well as reduce engine-out NOx and PM emissions by 15% and 42%, respectively. Engine out CO and HC emissions are still higher compared to CDC, but they are slightly reduced compared to dual mode operation with the original transmission controls. While altering the transmission controls for this theoretical study helps reveal the potential benefits of RCCI, it...
would clearly be desirable to expand the RCCI speed-load range as much as possible so that it could be more generally applicable to a range of drive cycle conditions. Therefore it is important to consider the impact of both strategies in future investigations.

5. Conclusions
Simulations of an RCCI-enabled light-duty diesel vehicle indicate that the engine-out NOx emissions can be reduced as much as 21% compared to conventional operation. However, the NOx benefits of RCCI as it is currently constrained can be much less, depending on the drive cycle. The chief barrier to achieving greater NOx reductions from RCCI is the current limitation on its speed and load operating range. Even if RCCI utilization continues to be constrained to certain speeds and loads, it appears that modification of transmission controls might make it possible to achieve more effective utilization of RCCI, thereby benefitting both fuel economy and NOx control.

Along with reductions in engine-out NOx, our simulations indicate that engine-out emissions of HCs and CO will be greatly increased with RCCI. This implies that robust catalytic oxidation aftertreatment will be more important when RCCI is used. Reductions in engine-out exhaust temperature during RCCI operation also imply that ensuring sufficient catalytic aftertreatment activity and utilization of exhaust heat (e.g., in waste heat recovery) will be more challenging.

The use of modified pistons for the RCCI measurements in this study complicates the comparisons between CDC/RCCI and CDC-only operation. This needs to be accounted for in future studies by reconstructing CDC-only maps using exhaust measurements from the engine with only the RCCI modified pistons. Future simulations also need to account better for more realistic transient dynamics when switching between RCCI and CDC operation.

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