

Combustion Simulation of Dual Fuel CNG Engine Using Direct Injection of Natural Gas and Diesel

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ABSTRACT

The increased availability of natural gas (NG) in the U.S. has renewed interest in the application to heavy-duty (HD) diesel engines in order to realize fuel cost savings and reduce pollutant emissions, while increasing fuel economy.

Reactivity controlled compression ignition (RCCI) combustion employs two fuels with a large difference in auto-ignition properties to generate a spatial gradient of fuel-air mixtures and reactivity. Typically, a high octane fuel is premixed by means of port-injection, followed by direct injection of a high cetane fuel late in the compression stroke. Previous work by the authors has shown that NG and diesel RCCI offers improved fuel efficiency and lower oxides of nitrogen (NO_x) and soot emissions when compared to conventional diesel diffusion combustion. The work concluded that NG and diesel RCCI engines are load limited by high rates of pressure rise (RoPR) (>15 bar/deg) and high peak cylinder pressure (PCP) (>200 bar). A high degree of premixing has been found by several researchers to cause excessively high rates of pressure rise thus limiting load.

The dual fuel engine proposed in this work employed direct injection of natural gas (DI-NG) (modeled as methane), as the main fuel, during the compression stroke in addition to early and late injections of small quantities of diesel fuel (modeled as n-heptane) to provide the ignition source. The DI-NG concept creates enhanced stratification of the NG fuel portion and avoids excessive premixing, which tempers the RoPR, thus enabling higher load operation.

A computational study was performed to examine the trade-offs of fuel consumption, PCP, and peak RoPR, with engine emissions. Several parameters were studied including: relative azimuthal angle between NG and diesel fuel nozzles, diesel pilot injection timing and quantity splits as well as injection timing sweeps. The results from the study indicated that DI-NG was successful in controlling the RoPR to below 10 bar/deg and PCP to less than 180 bar, while improving the NO_x, HC and soot emissions to meet engine out targets for engines equipped with modern aftertreatment systems.

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INTRODUCTION

Modern HD diesel engines use a combination of EGR and SCR for NO_x control, while high pressure fuel injection as well as diesel particulate filters are used for soot control. Each of these technologies adds cost and complexity to the engine while potentially increasing fuel consumption. EGR usage in HD diesel engines results in a well-known NO_x versus soot trade-off and requires a higher capacity air system placing additional demands on EGR cooling. SCR can reduce the amount of EGR necessary to attain low tail-pipe out NO_x emissions, but requires the use of urea which increases the operating costs and maintenance for the engine. Dual fuel DI-NG has the potential to eliminate or reduce the SCR requirement and reduce the demand for ultra-high fuel injection pressures.

Premixed compression ignition combustion engine concepts (e.g., HCCI, PCCI) circumvent the soot versus NO_x trade-off associated with conventional diesel combustion. This is because premixing eliminates fuel-rich, soot producing combustion zones allowing high rates of EGR to be used to control NO_x emissions. However, controlling the rate and phasing of heat release using these combustion strategies has proved to be very challenging [1, 2, 3].

The RCCI combustion strategy introduces the notion that overall reactivity of the fuel mixture can be varied to provide additional control over the rate and phasing of the heat release event. RCCI has been developed using various fuel combinations for the low and high reactivity fuels [4, 5, 6, 7, 8, 9, 10, 11]. The characteristic of the concept are to employ two fuels with large differences in reactivity

(e.g., gasoline and diesel) and tailor the injection strategy to generate in-cylinder spatial gradients of mixture concentration and reactivity. Port injection of the low reactivity fuel (premixed) and late direct injection of diesel fuel (stratified) is one way to realize this concept. The combustion proceeds from the high reactivity regions to low reactivity regions, thereby avoiding excessively high rates of pressure rise. The burn durations tend to be shorter than that of conventional diesel combustion, which results in reduced fuel consumption.

The RCCI concept with premixed NG, previously studied by the authors [12], utilized port-injected NG (assumed to be homogeneously mixed at the start of the simulation) and direct injections of diesel, similar to the comprehensive computational study of Nieman et al. [13]. RCCI differs from the high pressure direct injection (HPDI) or diesel pilot-ignited natural gas concept of Hill et al., which injects a single diesel pilot before TDC followed closely by direct injection of NG to generate a NG diffusion flame [14].

Dual fuel DI-NG is a further progression of RCCI with the aim of reducing the peak RoPR and further extending operating range. DI-NG along with multiple diesel injections differs from HPDI. With HPDI there is a single injection of a small diesel quantity to provide ignition for a subsequent single main NG fuel direct injection, resulting in NG mixing controlled combustion. DI-NG has one or two main NG injections during the compression stroke along with two or more diesel injections during the compression stroke to provide a spatial gradient in reactivity and ignition source while avoiding excessive premixing.

In this study, a combustion strategy was developed using DI-NG for a 15L HD diesel engine described in Table 1. A high power condition (1800rpm and 18bar BMEP) was used to make the comparisons between conventional diesel combustion, previous RCCI work (shown as Premixed NG) and the current DI-NG work. The number of injections, injection timing, and fuel quantity splits for the diesel fuel were varied. In addition, the relative global amount of diesel and NG was also considered. Comparisons between the various cases were based on gross indicated specific fuel consumption (gross ISFC) calculated over the valves closed portion of the cycle. Additionally, pollutant emissions (NO_x, soot, unburned HC and CO), PCP and peak RoPR are used for comparison.

Table 1. Engine description and operating conditions

Engine Speed (RPM)	1800
BMEP (bar)	18
Compression Ratio	16.2
Bore (mm)	137.2
Stroke (mm)	171.5
EGR (%)	36.5
AFR	19.8
Intake Manifold Pressure (bar,abs)	3.34
Temperature at IVC (K)	405
Diesel fuel injection nozzle	7 x 218 μ m
Diesel injection pressure (bar)	up to 1800
Fuel nozzle included angle (deg)	120 (baseline diesel) 150 (diesel) 100 (NG) DI-NG case

TECHNICAL APPROACH

In order to meet U.S. 2010 EPA HD diesel emission standards of 0.2 gNO_x/bHPPhr [15], modern HD diesel engines generally employ modest levels of EGR 15-20 % and are calibrated to emit approximately 1.0 gNO_x/bHPPhr engine-out and utilize SCR technology to provide the 80-90 % NO_x reduction required to achieve the mandate. By employing higher EGR levels (~36%) and lowering the engine-out NO_x level to 0.5 gNO_x/bHPPhr and combining with SCR after-treatment, the amount of urea needed can be reduced while the fill interval can be increased thus lessening the burden and cost on the operator.

In previous work, RCCI using multiple diesel injections (modeled as n-heptane) was employed to generate spatial gradients in reactivity prior to ignition of premixed NG (modeled as methane) and used to control the heat release rate [12].

The main limitations of RCCI were high PCP in excess of 200 bar and high peak RoPR greater than 15 bar/deg at 18 bar BMEP, which was found to be due to high premixing of NG.

A dual fuel strategy was conceived to mitigate the RCCI problem of high RoPR caused by excessive NG premixing. Figure 1 below provides an illustrative comparison of three dual fuel injection strategies; RCCI, HPDI and DI-NG.

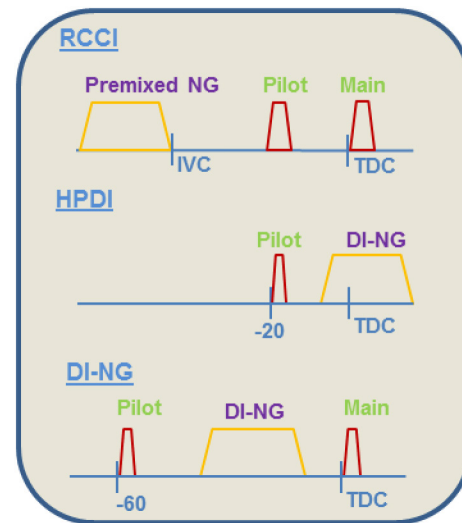


Figure 1. Dual fuel injection strategies (NG and Diesel)

The NG injection was moved from intake manifold into the cylinder by means of a secondary direct gaseous injection (DI-NG) to accompany the two direct diesel injections. The injector hardware envisioned could accomplish this by means of a single dual fuel coaxial injector using two separate injections paths with independently controlled actuation for each of the valves to meter the fuel flow. This would enable DI-NG during the compression stroke in addition to DI of small diesel fuel quantities.

It is believed, that by injecting during the compression stroke the NG fuel would avoid excessive premixing and thus would help enable control over the heat release leading to decreased peak RoPR and lower PCP. The initial DI-NG concept was limited to a single DI-NG

injection and two diesel injections for simplicity. The DI-NG injection occurs during the compression stroke sufficiently late enough to avoid excessive premixing. The first diesel injection is located anywhere during the compression stroke, whereas the second diesel injection should be located close to top dead center to control the start of combustion.

COMPUTATIONAL MODEL

The computation fluid dynamics code used for this study was KIVA-3V release 2 [16] coupled with CHEMKIN II for chemical kinetics calculations. Several improvements have been made to both the physical and chemistry models in the original KIVA-3V code [17, 18, 19, 20, 21]. The reduced ERC n-heptane mechanism [22] was used with 29 species and 52 reactions. NOx emissions were predicted using a reduced NO mechanism (4 species and 12 reactions) [23] and were added forming a new mechanism with a total of 33 species and 64 reactions. Natural gas was modeled as methane (CH₄) and the diesel fuel chemistry was modeled as n-heptane (C₇H₁₆) with the physical properties of diesel modeled as tetradecane (C₁₄H₃₀). Soot was predicted using the two-step phenomenological model based on the approach by Hiroyasu [24]. The acetylene (C₂H₂) species in the chemical kinetics mechanism was used as the soot pre-cursor species.

The liquid spray model uses the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach which models the fuel as numerical parcels containing drops that are coupled to the gaseous phase through the influence of drag. Droplet breakup was modeled using the hybrid Kelvin Helmholtz (KH) - Rayleigh Taylor (RT) model described by Beale and Reitz [19]. The droplet collision model is based on O'Rourke's model, with a radius of influence method used to determine the possible collision partners and reduce mesh dependency [25]. Interactions between droplets and the wall were considered via a wall film sub-model [26,27].

Gaseous Injection Validation

For the high pressure gaseous injections, a Lagrangian particle approach was used. Modifications made to the computational model allow multiple gaseous and liquid injections with different fuel types. The model implementation follows the methodology described by Hessel [29] with exception of the turbulence length scale modification. For this work, the gas-jet model of Abani [30] was used to set the turbulent kinetic energy and length scale in the path of the gaseous injection. A more complete description of the gaseous injection model is included in [Appendix A](#).

The gaseous injection model was validated using the experimental data of Ouellette [31]. [Table 2](#) shows the conditions for the high pressure natural gas injections. A total of four cases were tested with different back pressures. All tests were conducted with an ambient pressure of 14.9 bar. [Figure 2](#) shows model predictions of the vapor penetration compared to the test results. Good agreement is seen for the penetration over the pressure ratios examined.

Table 2. Test Conditions for the gaseous injections [31].

	Pressure Ratio	p_{back} (bar)	p_0 (kg/m ³)	p_{amb} (bar)	d_{eq} (cm)
PR5.4	5.4	80.88	64.9	14.9	0.076
PR4.0	4.0	60.01	48.1	14.9	0.064
PR2.5	2.5	37.26	29.8	14.9	0.050
PR1.5	1.5	22.85	18.3	14.9	0.041

The major weakness of the gas-jet model is that it does not capture the effect of ambient in-cylinder flow (eg. Swirl, tumble) on the injection process. However, the swirl ratio used in this work was very low (SR 0.5) and thus it is believed that the influence would be minimal if any. The gas jet model was not validated for combustion emissions as there was an absence of published engine data for the DI-NG model and injection strategy proposed in this paper.

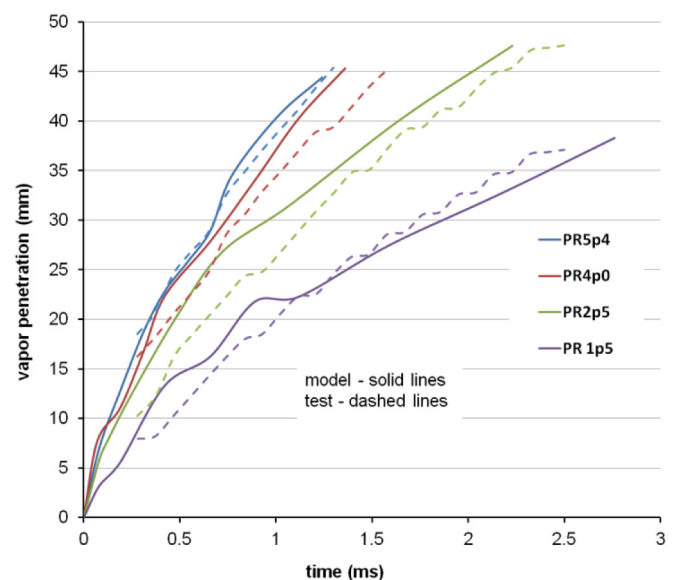


Figure 2. Vapor penetration for test (dashed) and model (solid) results.

Computational Mesh

A mesh consisting of a 51.42 degree sector of the 360 deg chamber is presented in [Figure 3](#). The mesh contains 35,600 cells at BTDC and uses periodic boundaries to model the valves closed portion of the engine cycle. To simplify the mesh, the crevice height was exaggerated to maintain the clearance volume at TDC. Only 1 injector nozzle each, for NG and diesel injections, is included in the sector mesh. The piston, cylinder liner and cylinder head wall boundaries were set to 575 K, 525 K, 575 K, respectively, with temperature at intake valve closing (IVC) set to 405 K with pressure at IVC a function of AFR, EGR and NG percentage.

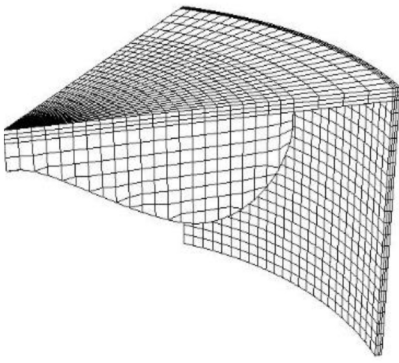


Figure 3. KIVA sector mesh

COMBUSTION SIMULATION RESULTS

The simulation study was conducted at 1800 rpm and a load of 18bar BMEP which corresponds to the C100 load point on the European Standard Cycle (ESC) 13-mode.

Simulation Input Boundary Conditions

The same AFR (19.8:1), EGR rate (36.5%), and compression ratio (CR 16.2) were used for this study as were used in a previous study for both the diesel baseline and premixed NG cases [12]. The in-cylinder IVC conditions were 405.5 K for both the diesel baseline and the DI-NG cases in this study whereas 380.9 K was used for the premixed NG case in the previous study. The simulation matrix for the DI-NG study is presented below in Table 3. Xg1 corresponds to the fuel mass fraction of total as gas whereas Xd1 and Xd2 correspond to the fuel mass fraction of total in first and second diesel injections respectively.

Table 3. Simulation Matrix for DI-NG study

Xg1 by mass	Xd1 by mass	Xd2 by mass	SOI _{g1} aTDC	SOI _{d1} aTDC	SOI _{d2} aTDC	SA g to d azimuthal deg
0.9	0.05	0.05	-20	-55 to -115	0	17.14
0.9	0.05	0.05	-20	-85	0	11.14 to 23.14
0.9	0.09	0.05 to 0.01	-20	-85	0	17.14
0.9	0.05	0.05	-26	-85	0 to -6	17.14
0.8	0.05 to 0.15	0.05	-20	-85	0	17.14

The total fuel (267 mg per cycle per cylinder) was split into two portions. The NG portion was set to 90% of the total fuel (in the base DI-NG case) and the diesel portion set to 10% of the total fuel resulting in 240.3 mg NG and 26.7 mg diesel fuel per cycle respectively. The diesel portion of the fuel was further split into pilot and main injection quantities.

Similar nomenclature is used for start of injection timing. SA g-to-d corresponds to the azimuthal angle between the gaseous and diesel sprays. For this study, the following key performance targets and limits were used:

- NO_x emissions: 2.0 g/kgfuel (~0.27 g/bHP_{hr})
- Soot emissions: 0.5 g/kgfuel (~0.07 g/bHP_{hr})
- Unburned hydrocarbons: 7.5 g/kgfuel (~1.0 g/bHP_{hr})
- Maximum rate of pressure rise: 10 bar/deg
- Peak cylinder pressure: 180 bar
- Gross ISFC: 176 g/kWhr

Diesel Pilot Injection Timing Sweep

Figure 4 presents the DI-NG gross ISFC versus SOI_{d1} compared to the premixed NG case and baseline diesel case.

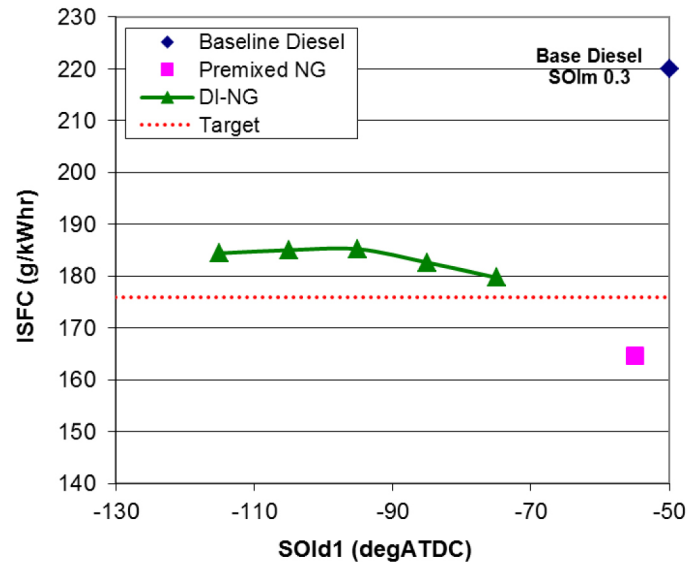


Figure 4. Gross ISFC versus start of injection timing of pilot diesel.

The base DI-NG injection strategy contains a single NG injection during the compression stroke containing 90% of total fuel and two diesel injections, pilot and main, each with 5% of the total fuel. The pilot diesel injection is located prior to the NG injection during the compression stroke whereas the second diesel injection is located close to TDC for ignition timing control.

The start of injection timing of the diesel pilot (SOI_{d1}) was swept from -75 to -115 degATDC in 10 degree increments. Note the base diesel case did not have a pilot injection. The DI-NG gross ISFC was higher with earlier injection timings. DI-NG cases had higher gross ISFC compared to the premixed NG case due to longer heat release durations and lower combustion efficiency.

The soot versus NO_x emissions for the pilot diesel timing sweep is plotted in Figure 5. Earlier diesel pilot injection timings resulted in reduced NO_x emissions and slightly reduced soot emissions for the DI-NG cases. This is due to the enhanced level of premixing of the diesel pilot fuel quantity. The premixed NG case and the DI-NG cases showed very low NO_x and soot to within target levels whereas the baseline diesel case had high soot.

The optimal pilot diesel injection was found to be at -85 degATDC in terms of meeting soot emissions and maintaining low gross ISFC (182 g/kWhr). The peak RoPR for the SOI_{d1} sweep of DI-NG (not shown) was found to be constant at 5 bar/deg. Similarly, the PCP (not shown) was similar to the baseline diesel case at approximately 155 bar. Unburned hydrocarbons (not shown) were excessively high in the range of 10 to 12 g/kgfuel, indicating poor combustion efficiency.

For the DI-NG cases, earlier diesel pilot injection timings result in reduced NO_x emissions, modestly decreased soot emissions, and modestly increased gross ISFC. Varying SOI_{d1} timings had little