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Physical and chemical effects of low octane gasoline fuels on compression ignition combustion

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HIGHLIGHTS

- New experimental data SOI sweep in GCI engine running on naphtha fuels.
- Despite the differences in the fuel's properties, the combustion and emissions were similar.
- CFD engine simulations successfully reproduced the experimental trends.
- The chemical and physical effects were isolated numerically and detailed analysis was performed.

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ABSTRACT

Gasoline compression ignition (GCI) engines running on low octane gasoline fuels are considered an attractive alternative to traditional spark ignition engines. In this study, three fuels with different chemical and physical characteristics have been investigated in single cylinder engine running in GCI combustion mode at part-load conditions both experimentally and numerically. The studied fuels are: Saudi Aramco light naphtha (SALN) (Research octane number (RON) = 62 and final boiling point (FBP) = 91 °C), Haltermann straight run naphtha (HSRN) (RON = 60 and FBP = 140 °C) and a primary reference fuel (PRF65) (RON = 65 and FBP = 99 °C). Injection sweeps, where the start of injection (SOI) is changed between −60 and −11 CAD aTDC, have been performed for the three fuels. Full cycle computational fluid dynamics (CFD) simulations were executed using PRFs as chemical surrogates for the naphtha fuels. Physical surrogates based on the evaporation characteristics of the naphtha streams have been developed and their properties have been implemented in the engine simulations. It was found that the three fuels have similar combustion phasings and emissions at the conditions tested in this work with minor differences at SOI earlier than −30 CAD aTDC. These trends were successfully reproduced by the CFD calculations. The chemical and physical effects were further investigated numerically. It was found that the physical characteristics of the fuel significantly affect the combustion for injections earlier than −30 CAD aTDC because of the low evaporation rates of the fuel because of the higher boiling temperature of the fuel and the colder in-cylinder air during injection.

1. Introduction

Around 40% increase in global transport energy demand is expected by the year 2040 according to energy projections [1–4]. Even with this increase in energy demand, more than 90% of the global transport energy demand is currently and is expected to continue be supplied by the petroleum-based liquid fuels such as gasoline, diesel, jet and heavy fuel oil fuels [2]. Therefore, improving the fuel efficiency at low cost in transportation sector can help not only saving the global energy usage but also reducing the greenhouse gas (GHG) CO_2 emissions.

Gasoline compression ignition (GCI) engines have recently emerged as a promising technology for diesel-like thermal efficiencies with significantly reduced engine-out nitrogen oxides (NOx) and soot emissions by achieving low temperature combustion (LTC) conditions [5]. Recent studies [6–10] reported that GCI combustion occurs as a series of autoignition events with minor contributions from flame fronts. The autoignition timing is controlled by manipulating the mixture composition and temperature

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Nomenclature

3D	three dimensional
ASTM	American Society for Testing and Materials
aTDC	after top dead center
BiCGSTAB	biconjugate gradient stabilized
CAD	crank angle degree
CFD	computational fluid dynamics
CO	carbon monoxide
COV	coefficient of variation
CR	compression ratio
DCN	derived cetane number
EGR	exhaust gas recirculation
ETC/ED	effective thermal conductivity/effective diffusivity
EVO	exhaust valve opening
FBP	final boiling point
FSN	filter smoke number
FTP	federal test procedure
GCI	gasoline compression ignition
GDI	gasoline direct injection
GHG	greenhouse gas
HC	hydrocarbon
HCCI	homogeneous charge compression ignition
HSRN	Haltermann straight-run naphtha
IMEP	indicated mean effective pressure
IQT	ignition quality tester
KH-RT	Kelvin-Helmholtz and Rayleigh-Taylor
LHV	lower heating value
LTC	low temperature combustion
MON	motor octane number
MPCI	multiple premixed compression ignition
NMEP	net mean effective pressure
NOx	nitric oxides
NTC	negative temperature coefficient
OI	octane index
PISO	Pressure Implicit with Splitting of Operators
PPCI	partially premixed compression ignition
PRF	primary reference fuel
RON	research octane number
RPM	revolutions per minute
SALN	Saudi Aramco light naphtha
SOI	start of injection
SOR	successive over-relaxation
TDC	top dead center
TPRF	toluene primary reference fuel

stratification within the cylinder through late injection in the compression stroke. This is in contrast to homogeneous charge compression ignition (HCCI) [11–15] and premixed ignition [16,17] engines where the fuel and air are fully mixed prior to entering the combustion chamber. Recently, a new engine combustion concept named "multiple premixed compression ignition" (MPCI) has been investigated as an option to increase efficiency and reduce pollutants [18–21] by manipulating the stratification of the charge to control the pressure rise rates.

The enabling fuels for such GCI, partially premixed compression ignition (PPCI) and MPCI combustion modes are generally in the gasoline boiling range. Compared to commercial gasoline and diesel fuels, refinery streams such as petroleum naphtha with low octane numbers (RON) in the 50–80 range have recently been considered attractive alternatives to provide suitable chemical characteristics (longer ignition delay than diesel) in GCI engines at lower production cost and well-to-tank CO_2 emissions. Hao et al. [22] found that compared with the conventional pathway, the low-octane gasoline-GCI pathway leads to a 24.6% reduction in energy consumption and a 22.8% reduction in GHG emissions. A naphtha stream with a RON of 65 was utilized in [18–21] to investigate the MPCI mode. They have also tested diesel and gasoline blends with the aim of reducing the ON to the 50–80 range. They have reported that the naphtha fuel can be used to cover wide operating load points while resulting in higher thermal efficiencies and lower emissions. Han et al. [10] also tested the combustion of diesel and gasoline blends in compression ignition mode. It is clear from literature that the properties (RON, MON, density, boiling range and ...) of the fuel that is suitable for PPCI or MPCI are not fully determined yet. Therefore, it is of interest to understand the effects of the fuel's physical and chemical properties on the combustion and emission behavior of petroleum naphtha in GCI conditions. Kim et al. [23] studied the effects of some physical properties (density, vapor pressure, viscosity, surface tension, heat of vaporization and specific heat capacity) in a reaction fuel sprays. They found that density, viscosity, heat of vaporization and specific heat had significant impact on liquid penetration length. They also reported that specific heat and density significantly affected the ignition delay of the system. Lacey et al. [24] also studied the effects of the properties of gasoline refinery streams on the auto-ignition quality of a fuel and the HCCI combustion. They have observed that the fuel composition significantly affects the combustion phasings of gasoline fuels with the same RON and MON. They have proposed a new octane index (OI) correlation that accounts for the aromatics, olefins, saturates and ethanol contents in the gasoline.

Full cycle computational fluid dynamics (CFD) simulations with detailed chemical kinetics and turbulent transport can also provide fundamental understanding of the spray development and stratification and their effects on the combustion process. Ra et al. [25] performed extensive numerical studies on GCI combustion to investigate the effects of injection parameters, gas temperatures, boost pressure and exhaust gas recirculation (EGR) on combustion characteristics such as combustion phasing and important emissions. Recently, Badra et al. [26] reported a numerical study on the optimization of the spray models for outwardly opening hollow cone spray and the effects of primary reference fuel (PRF) and toluene primary reference fuel (TPRF) chemical surrogates on the combustion phasing of GCI engine running on naphtha fuel. Another study [27] also investigated the mixing effects of a light naphtha stream on the combustion phasing of a compression ignition engine.

In this work, we investigate the effects of mixing and spray/piston interactions on the combustion phasing and emissions over a range of injection parameters using three carefully chosen low octane fuels. We first report new experimental data that investigate the effect of start of injection (SOI) on the combustion phasing and emissions in a GCI engine running on three fuels with different chemical and physical characteristics. Full-cycle GCI engine 3D CFD simulations using different chemical and physical surrogate fuels are then presented and validated with experimental data. Subsequently, the simulation data are thoroughly investigated through detailed equivalence ratio-temperature (Φ-T) for carefully chosen fuels with different chemical and physical properties, in order to provide insights into the observed engine combustion behavior.