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Full Length Article

A Computational investigation of the potential for non-sooting fuels to enable ultra-low NOx and CO_2 emissions

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ABSTRACT

Lean and stoichiometric DME fueled compression ignition engine concepts were compared to a base heavy-duty diesel engine at the near rated power operating condition. The ability to achieve ultra-low emissions and high thermal efficiency was evaluated using a combined 3D CFD and 1D cycle simulation approach. The peak gross indicated efficiency was achieved using lean DME operation due to improvements in mixing resulting from the DME injection event. Stoichiometric operation resulted in reductions in gross indicated efficiency due to incomplete combustion. System level comparisons showed that, when the impact of NOx after-treatment, air handling, and waste heat recovery are considered, the stoichiometric DME cases show an improvement in efficiency over lean DME and lean diesel combustion. The improvements are the result of reductions in pumping losses, elimination of DEF losses, and recovery of exhaust energy. Well-to-wheels analysis was performed and CO_2 emission showed a heavy dependence on fuel feedstock for DME. Finally, extreme downsizing was investigated and it was found that stoichiometric operation provides the potential to decrease the displacement by a factor of two with no degradation in power, similar brake thermal efficiency, and near zero NOx emissions.

1. Introduction

Future proposed NOx emissions regulations pose a significant challenge for heavy-duty (HD) compression ignition (CI) engines even when considering advancements in lean NOx after-treatment (e.g., selective catalytic reduction (SCR) systems). In recent years, a substantial effort has focused on enabling high efficiency and low emissions using advanced combustion. For example, Dec [1] demonstrated high efficiency and low NOx and soot emissions across a wide range of conditions using gasoline homogenous charge compression ignition (HCCI) combustion. The results are promising, but controlling HCCI combustion, especially at high engine loads, is challenging. Additionally, to enable combustion at full load conditions, they needed greater than 50% external exhaust gas recirculation (EGR) to lengthen chemistry timescales to avoid overly advanced combustion phasing. This high level of EGR, coupled with the associated high intake pressure requirement, may offset the gross efficiency benefits and result in reduced overall system efficiency, as demonstrated by Chadwell et al. [2]. To address the issue of combustion phasing control with advanced combustion, Kokjohn et al. [3] proposed blending two fuels inside the combustion chamber to control the rate of heat release. Similar to the efforts by Dec and others, their results showed that highly premixed CI operation shows promising efficiency and emissions characteristics, but a high level of EGR is required to enable high load operation [4,5].

An alternative approach to enable low NOx emissions without the need for a secondary fluid and the added cost associated with lean NOx after-treatment is the use of stoichiometric operation coupled with a three-way catalyst (TWC). When stoichiometric operation is maintained, the NOx conversion efficiency of TWCs is nearly 100% [6]. However, when the equivalence ratio is leaner than stoichiometric the NOx conversion efficiency decreases rapidly [7]. Accordingly, several researchers have investigated stoichiometric CI engine operation to leverage the efficiency advantages of CI engines, while maintaining the ultra-low NOx emissions of a TWC equipped spark-ignition engine [8,9].

With conventional fuels, stoichiometric operation presents challenges due to excessive soot formation. For example, Windsor and Baumgard [10] investigated stoichiometric diesel fueled operation and found soot levels were increased an order of magnitude above typical diesel operation values. Use of oxygenated fuels is a potential pathway to address the high soot levels of diesel fueled stoichiometric engines. Miyamoto et al. [11] investigated sooting tendencies of fuel as a function of fuel oxygen concentration and found that fuels with greater than 30% oxygen, by mass, produced negligible soot. Roberts et al. [12] proposed a high temperature combustion methanol or ethanol fueled CI engine and showed that both methanol and ethanol produced near zero

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Nomenclature

AFR	air fuel ratio
AHRR	apparent heat release rate
ATDC	after top dead center
BDC	bottom dead center
BMEP	brake mean effective pressure
BTE	brake thermal efficiency
CDC	conventional diesel combustion
CFD	computational fluid dynamics
CI	compression ignition
DEF	diesel exhaust fluid
DME	di-methyl ether
DPF	diesel particulate filter
EGR	exhaust gas recirculation
ERC	Engine Research Center
EVO	exhaust valve opening
FMEP	friction mean effective pressure
GIE	gross indicated efficiency
GREET	Greenhouse gases, Regulated Emissions, and Energy in Transportation
GRI	Gas Research Institute
HCCI	homogenous charge compression ignition
HD	heavy-duty
IMEP	indicated mean effective pressure
IVC	intake valve closing
KH	Kelvin-Helmholtz
LDEF	Lagrangian drop Eulerian fluid
NIE	net indicated efficiency
PM	particulate matter
PMEP	pumping mean effective pressure
RNG	re-normalization group
RT	Rayleigh-Taylor
SCR	Selective catalytic reduction
SOI	start of injection
TDC	top dead center
TFBTE	total fluid brake thermal efficiency
TWC	three-way catalyst
WHR	waste heat recovery
WTT	well-to-tank

levels of soot even at stoichiometric conditions. Although the methanol and ethanol results are promising, cold-starting and low load operation may present a challenge. An alternative approach is to use a high-cetane, high oxygen concentration fuel. One example is di-methyl ether (DME) [13,14]. Previous research using DME as a CI engine fuel has shown the potential to significantly reduce engine-out soot and eliminate the need for soot after-treatment [15,16]. For example, Szybist et al. [17] compared particulate matter (PM) from DME fueled and diesel fueled engines. They showed that the DME engine system produced lower levels of PM without after-treatment than the diesel particulate filter (DPF) equipped diesel-fueled engine. Kim et al. [18] investigated the use of DME in a CI engine and found higher thermal efficiency and lower CO emissions compared to the same engine operated on diesel fuel. Kim and Park [19] performed a computational optimization of a DME fueled engine and compared the results to baseline diesel operation. They found that, once both strategies were optimized, DME combustion allowed lower NOx levels than conventional diesel combustion. However, they showed that to meet current NOx regulations, injection timing had to be retarded beyond top dead center, likely lowering thermal efficiency. This work suggests a coupled approach combining NOx after treatment and DME fueled engine operation may enable simultaneous improvements in system level thermal efficiency and reductions in tailpipe NOx emissions.

In addition to enabling very low soot emissions and stoichiometric operation, DME can be produced from a variety of conventional and renewable sources [20,21]. For example, DME may be synthesized from natural gas through a variety of processes [22]. It may also obtained by synthesis from bio-based feedstock yielding very low well-to-tank CO_2 emissions [23].

2. Approach

The present work investigates DME as an oxygenated fuel to enable near zero NOx and soot emissions using stoichiometric CI operation. The near rated power operating condition of a HD diesel engine was studied using a combined 3-dimensional (3D) computational fluid dynamics (CFD) and 1-dimensional (1D) cycle simulation approach. Simplified approaches to include the impact of air handling, exhaust after-treatment, and waste heat recovery devices are considered to present a pathway to enable system level efficiency improvements while achieving system level NOx at sub-ppm levels. The target NOx of the present effort is 0.0268 g/kW-hr based upon potential future NOx emissions regulations proposed by CARB [24]. Comparisons are made to conventional diesel operation and lean DME operation. The potential to further improve system level efficiency is evaluated by analyzing the potential for extreme downsizing using stoichiometric DME operation.

3. Methods

3.1. Multi-Dimensional computational fluid dynamics modeling

Closed cycle simulations (i.e., from intake valve closure (IVC) to exhaust valve opening (EVO)) of the spray, mixing, and combustion process were performed using an in-house CFD code based on the KIVA family of codes. The code includes improved physical and chemistry models developed at the University of Wisconsin's Engine Research Center (ERC) [25]. The spray model used the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach. In order to reduce the grid size dependency of the LDEF spray model and allow accurate spray simulation in the near nozzle region, the Gasjet model of Abani et al. [26,27] was used to model the relative velocity between the droplets and gas phase in the near nozzle region. The Kelvin Helmholtz-Rayleigh Taylor (KH-RT) model was used to model the spray break-up [28]. The Re-Normalization Group (RNG) k-ε model was used for the turbulent flow calculation [29]. The droplet collision model was based on O'Rourke's model and was expanded by Munnanur [30] to include a comprehensive list of collision outcomes that considers effects of bounce, coalescence, and fragmenting and non-fragmenting separations. A wall film sub-model was used to model droplet interaction with wall [31].

The code was coupled with CHEMKIN II for chemical kinetics calculations. The well-stirred reactor approach was used. Diesel fuel

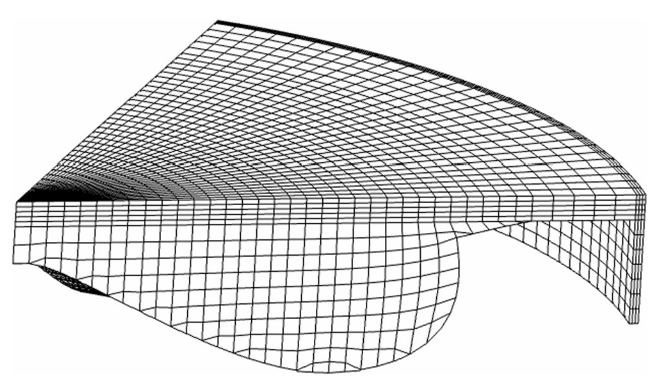

Fig. 1. Computational sector mesh shown at top dead center (TDC).