Fuel 223 (2018) 20–31

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Computational optimization of a combustion system for a stoichiometric DME fueled compression ignition engine

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ARTICLE INFO

Keywords:
Diesel engine
Alternative fuels
Pollutant emissions
Engine efficiency
Engine optimization
Three way catalyst
Stoichiometric combustion

ABSTRACT

An optimization methodology based on a genetic algorithm coupled with the KIVA computational fluid dynamics (CFD) code is applied to the design of a combustion system of a heavy-duty diesel engine fueled with dimethyl ether (DME) and working with stoichiometric combustion in order to equip the system with a three way catalyst (TWC) to control the NOx emissions. The target of the optimization is to improve net indicated efficiency (NIE) while keeping NOx emissions, peak pressure and pressure rise rate under the reference engine levels. The results of the study provide an optimum configuration that offers a 0.6% NIE improvement while satisfying the restrictions and offering NOx values lower than 1% of the original emissions. Due to the methodology, not only the optimum combustion system configuration is presented, but also the cause-effect relation of the most relevant inputs with the optimization outputs are identified and analyzed. The new geometry shape reduced heat transfer losses by minimizing the surface area. Injection pressure and swirl proved to be key parameters necessary to overcome the increased mixing requirements of stoichiometric operation. EGR was found to simultaneously increase NIE while controlling NOx emissions. The results show the potential of stoichiometric compression ignition operation using DME as a promising pathway to maintain diesel-like efficiency, while achieving near zero NOx and soot emissions.

1. Introduction

Recent research on combustion systems, especially those applied to road and rail transport applications, is focused on improving the fuel consumption while keeping the pollutants under the regulation standards. Diesel (compression ignition) engines are one of the most efficient engines in the world. They are known as economical and robust, but also for their smoke and NOx emissions levels [1]. Different emissions control strategies can be used to control pollutant depending if they are applied during or after the combustion process. The techniques applied directly to the combustion process include Low Excess Air (LEA) burn [2] and Exhaust Gas Recirculation (EGR) [1,3]. EGR is a widely used technique to control NOx emissions; however, high levels of EGR have a noticeable impact on engine efficiency and particulate matter emissions, forcing the research community to find new ways to further control NOx. Current production diesel engines are often equipped with Selective Catalytic Reduction (SCR) or a Lean NOx Trap (LNT) for post-treatment of NOx in the exhaust stream [4]. Although SCR and LNT systems can effectively control NOx emissions, challenges with these systems warrant exploration of alternative methods for emissions control. LNT systems struggle to reach the high NOx conversion efficiencies required to meet current and future regulations over the wide range of conditions experienced during engine operation [5]. Additionally, LNT systems often increase fuel consumption due to periodic rich operation required for regeneration. Urea SCR systems typically have much higher NOx conversion efficiency than LNT

Definition of Acronyms: ATDC, After Top Dead Center; ACT, apparent combustion time; CAD, Crank Angle Degree (degrees to top dead center); CARB, California Air Resources Board; CFD, computational fluid dynamics; CO, carbon monoxide; COSSO, Component Selection and Smoothing Operator; DEF, diesel exhaust fluid; DME, dimethyl ether; Dnoz, nozzle hole diameter; dS, cell size; EGR, exhaust gas recirculation; ERC, Engine Research Center; EVO, exhaust valve opening; GA, genetic algorithm; HCCI, homogenous charge compression ignition; HD, Heavy Duty; HRR, heat release rate; IMEP, gross indicated mean effective pressure; IP, injection pressure; IVC, intake valve closure; KH, Kelvin Helmholtz; LDEF, Lagrangian-Drop and Eulerian-Fluid; LEA, Low-Excess-Air; LNT, Lean-NOx-Trap; maxPRR, maximum pressure rise rate; NA, nozzle angle; NIE, net indicated efficiency; NSGAII, non-dominated sorting genetic algorithm; PIVC, pressure at IVC; PP, peak cylinder pressure; RCCI, Reactivity Controlled Compression Ignition; RSM, root-mean-square; RT, Rayleigh Taylor; SCR, selective catalytic reduction; SOI, start of injection; TWC, three way catalyst; UHC, unburned hydrocarbons; WSR, Well Stirred Reactor

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https://doi.org/10.1016/j.fuel.2018.03.022
Received 12 June 2017; Received in revised form 1 March 2018; Accepted 5 March 2018

systems (conversion efficiencies can be in the range of 90–95%); however, diesel exhaust fluid (DEF) dosing required for NOx reduction may increase the overall operational cost compared to a non-SCR equipped engine. Additionally, SCR systems struggle to achieve high NOx conversion efficiencies at temperatures below approximately 200 °C due to deposit formation from DEF dosing [6] and poor catalyst activity [7]. Currently, SCR equipped heavy-duty diesel engines are capable of meeting current regulated NOx emissions limits on the order of 0.268 g/kWh. However, the California Air Resources Board (CARB) has proposed future NOx targets of 0.0268 g/kWh [8]. Reaching this level of tailpipe NOx with a urea SCR system will likely be challenging. That is, NOx conversion efficiencies would need to be on the order of 99%.

An alternative approach to enable low NOx emissions is the use of stoichiometric operation coupled with a three way catalyst (TWC). The TWC is a widely used technique, is low cost, and can reach a NOx reduction over 99% [9]. The drawback is that, because stoichiometric operation is required, use with diesel fueled engines has resulted in extremely high soot emissions [10–12]. An alternative approach is to couple stoichiometric operation with a low sooting fuel. One such fuel is dimethyl ether (DME). DME has comparable combustion characteristics to those of diesel fuel [13], but produces no soot emissions even under stoichiometric operation [14–16].

The literature shows some previous research in the field of engines fueled with DME that shows the potential of the fuel. An optimization of a DME fueled engine with the micro-genetic algorithm was performed by Hyung et al. [17]. The results demonstrated the advantage of the non-sooting nature of DME fuel that allows breaking the NOx-soot trade-off that affects diesel engines just optimizing engine settings. For that reason, new strategies for low NOx emissions and high efficiency can be tested with the new fuel that would not be possible to apply to a diesel fueled engine due to soot restrictions. These conclusions were tested experimentally by Park et al. [18]. Further work has been done including a piston geometry coupled with injection settings optimization by Park et al. [19]. The optimum geometry was shifted from the conventional diesel reentrant shape to a bathtub type shape coupled with earlier SOI, designing a new combustion chamber with lower emissions without efficiency penalization. An equivalent optimization was also performed for the original engine fueled with diesel and the results present an optimum with lower emissions, but an unavoidable increase in fuel consumption, proving the potential of DME compression ignition operation.

In the present study, we take advantage of the non-sooting nature of DME and apply a TWC in order to achieve future pollutant regulation standards. Under stoichiometric operating conditions, it is expected that complete oxygen utilization will be challenging, potentially requiring changes to the combustion system geometry (e.g., piston bowl shape). The present study computationally optimizes a combustion system for a Heavy Duty (HD) compression ignition engine fueled with DME working with stoichiometric combustion and presents a pathway to maintain diesel-like efficiency while meeting future NOx targets.

2. Methods

2.1. Experimental setup

The engine used is a single cylinder version of a Caterpillar C-15, 15-L six-cylinder engine. Table 1 shows the engine and injector specifications. The C-15 is typical of a heavy-duty size-class diesel engine with a bore of 137 mm and a stroke of 171 mm yielding a displacement of 2.5 L per cylinder.

The engine was operated at 1800 rev/min and a nominal load of 18 bar gross indicated mean effective pressure (IMEP) (i.e., near the rated power condition). For the validation tests carried out using diesel fuel, the fueling was held constant and the SOI timing was swept from −18 to −3 deg aTDC. The EGR rate, intake pressure, and intake temperature were held constant at 25%, 3.1 bar, and 60 °C, respectively. Details of the operating condition and its related settings are included in Table 2.

Table 1
Engine and injector specifications.

Engine Specifications	
Displacement [L/cylinder]	2.5
Bore × Stroke [mm]	137 × 171
Compression Ratio [–]	17:1
Swirl Ratio [–]	0.7
IVC [deg aTDC]	−154
EVO [deg aTDC]	113
Fuel Injector	
Number of Holes	6
Hole Diameter [mm]	0.214
Included Spray Angle [deg]	130

Table 2
Operating conditions for model validation experiments [20].

Nominal gross IMEP [bar]	18
Speed [rpm]	1800
Intake Temperature [K]	333
Coolant Temperature [K]	353
EGR Temperature [K]	333
Intake Pressure [bar]	3.1
SOI Timing – command [deg aTDC]	−18 to −3
Fuel Mass [mg/cycle]	252
EGR Rate [%]	25
Motored Temperature at TDC [K]	1018
Motored Pressure at TDC [bar]	147
Injection Pressure [bar]	1800
Fuel	Halterman Certification Diesel

2.2. Computational approach

Computations were performed using an in-house computational fluid dynamics code based on the KIVA-3v release 2 platform [21] with improvements to many physical and chemistry models developed at the Engine Research Center (ERC) [22–24]. To reduce computing time, simulations consider a sector of the combustion chamber, representing a single nozzle hole of the six hole fuel injector. Additionally, the simulations are restricted to the closed engine cycle, from intake valve closure (IVC) to exhaust valve opening (EVO). The simulations were initialized using solid body rotation to specify the azimuthal velocity flow field at IVC. This section provides an overview of the physical models important to the present study.

2.2.1. Combustion model

The KIVA-3v code is coupled with the SpeedCHEM [25] solver for detailed chemistry calculations. The RNG k-ε model [26] is used for the turbulence calculations; however, sub-grid turbulence-chemistry interactions are not considered. That is, the current implementation of the SpeedCHEM solver considers every computational cell to be a Well Stirred Reactor (WSR) and the cell average species production rates are assumed to be equal to the species production rates evaluated at the average cell conditions. At each time step, species concentrations and thermodynamic conditions are passed to the chemistry solver for each computational cell. The chemistry solver then integrates the mass and energy equations at constant volume over a period of time equal to the computational time step. Although, sub-grid scale turbulent-chemistry interactions are not considered, by coupling the chemistry solver with the CFD code, the effects of turbulence on combustion are accounted by modeling the effects of turbulence on property transport, heat flux, and mixture formation. Justification for this modeling approach has also been discussed by Kokjohn and Reitz [27].

The chemistry of dimethyl ether was simulated using a reduced