KNOCK IN DUAL-FUEL DIESEL COMBUSTION WITH AN E85 ETHANOL/GASOLINE BLEND BY MULTI-DIMENSIONAL SIMULATION

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(Received 8 May 2015; Revised 4 January 2016; Accepted 6 January 2016)

ABSTRACT – In this paper, knocking combustion in dual-fuel diesel engine is modeled and investigated using the CFD code coupled with detailed chemical kinetics. The ethanol/gasoline blend E85 is used as the primary fuel in a dual-fuel combustion concept based on a light-duty diesel engine equipped with a common-rail injection system. The E85 blend is injected and well mixed with intake air in the intake manifold and is ignited by the direct injection diesel fuel. A 46-species, 187-reaction Multi-component mechanism is adopted to model the auto-ignition process of the E85/air/diesel mixture ahead of the flame front. Based on the model validation, knocking combustion under boost and full load operating condition for 0 %, 20 %, 50 %, as well as 70 % E85 substitute energy is simulated. The effects of E85 substitute rate and two stage injection strategies on knock intensity, power output, as well as location of the auto-ignition initiation is clearly reproduced by the model. The calculation result shows that, for a high E85 rate of 50 % and 70 % with single injection strategies, the most serious knock and the origin of auto-ignition always occurs far away from where the flame of diesel spray is first generated, at the center of combustion chamber, due to higher pressure wave, relatively richer E85 mixture and longer distances of flame propagation. The two stage injection strategies with a small amount of diesel pilot injection ahead of the main injection primarily influence the ignition behavior of the directly injected fuel, leads to a lower pressure rise rate and a reduced propagation distance, both of which contribute to the attenuation of knock intensity for a higher E85 rate.

KEY WORDS : Dual-fuel, Ethanol, Knock, Simulation, Detailed chemical kinetics

NOMENCLATURE

ABDC : after bottom-dead center
ATDC : after top-dead center
BTDC : before top-dead center
CA : crank angle
CFD : computational fluid dynamics
CO : carbon monoxide
DISI : direct injection spark-ignition
DF : dual-fuel
DME : dimethylether
EGR : exhaust gas recirculation
ECFM : extended coherent flamelet model
EVO : exhaust valve opening
HC : hydrocarbon
HRR : heat-release rate
IVC : intake-valve closing
KI : knock index
LNG : liquefied natural gas
MultiChem : multi-surrogate fuel chemistry
NG : natural gas
PDF : probability density function
PI : power index
PPmax: maximum amplitude of pressure oscillations

PRF : primary reference fuel
PRR : pressure rise rate
RON : research octane number
SOI : start of injection
TDC : top-dead center
THC : total unburned hydro-carbon

1. INTRODUCTION

With the increase of energy crisis and climate change, the outlook of world energy markets which are among the most important factors influencing economic and industrial development has changed fundamentally during the last few years. Main technical challenges against upcoming diesel engines are the enforcement for complying with highly stringent emission standard while retaining benefit in fuel economy over its competitor, spark ignition engines. The introduction of expensive and complicated after-treatment systems will deteriorate competitiveness of future diesel engines (Feng and Lü, 2015; Lee et al., 2015a). The main concerns for moving towards cleaner, more efficient and alternative energy sources have been the dwindling fossil fuel reserves and the more stringent vehicles emission regulations (IEA, 2010, 2011). Ethanol is regarded as one of the feasible solutions for addressing the concerns because of its renewable features and peculiar

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Table 1. Fuel properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Diesel</th>
<th>Ethanol</th>
<th>Gasoline</th>
<th>E85</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower heating value (MJ/kg)</td>
<td>43.2</td>
<td>26.8</td>
<td>42 ~ 45</td>
<td>28.7</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>840</td>
<td>789</td>
<td>735 ~ 760</td>
<td>784</td>
</tr>
<tr>
<td>Research octane number (RON)</td>
<td>15 ~ 25</td>
<td>108.6</td>
<td>93</td>
<td>105</td>
</tr>
<tr>
<td>Cetane number</td>
<td>53</td>
<td>5 ~ 8</td>
<td>0 ~ 10</td>
<td>-</td>
</tr>
<tr>
<td>Vapour pressure (kPa)</td>
<td>45 ~ 90</td>
<td>18</td>
<td>54.7 ~ 60.8</td>
<td>54.3</td>
</tr>
<tr>
<td>Heat of vaporisation (kJ/kg)</td>
<td>310</td>
<td>904</td>
<td>340 ~ 370</td>
<td>850</td>
</tr>
<tr>
<td>Boiling point (°C)</td>
<td>180 ~ 360</td>
<td>78.4</td>
<td>25 ~ 215</td>
<td>84.8</td>
</tr>
</tbody>
</table>

physical-chemical properties (Wu et al., 2011; Sarathy et al., 2014). E85 is a liquid blend of ethanol and gasoline and contains a maximum of 85 % ethanol by volume. E85 is widely available in many countries (e.g. Brazil and USA) due to the simpler distribution and storage infrastructure (Padala et al., 2013b). The physical and chemical properties of gasoline, Ethanol, and E85 are listed in Table 1.

Ethanol blended combustion in a SI engine has great potential to enhance engine anti-knock ability (Costa and Sodré, 2011; Celik, 2008), to achieve higher efficiency and low unburned emissions such as hydrocarbon (HC) and carbon monoxide (CO) (He et al., 2003; Poulopoulos et al., 2001). However, a drawback of the vehicles is the ignition problems during cold start (Chen et al., 2011) due to the high heat of vaporization and a low vapor pressure of ethanol (Padala et al., 2013a). More importantly, small amounts of water in ethanol will cause phase separation, which incurs higher costs in the purification process (Demirbas, 2000). In addition, ethanol can be used in higher compression ratio engines due to a much higher resistance to knock (Padala et al., 2013b), and the problems of corrosion and reduced lubrication still exist in these vehicles (Kabasin et al., 2009). Previous studies have found that these issues can be addressed in a dual-fuel diesel engine with two separate fuel injection systems (Tsang et al., 2010; Rodriguez-Fernández et al., 2009; Ogawa et al., 2010), which deliver ethanol in the intake manifold and directly inject diesel into the cylinder. The cold-start issue can also be addressed with diesel-only combustion during the warm-up period. Also, Water in ethanol is not so problematic if there is no blending. Ethanol can be burned in diesel engines with higher compression ratio, which result in higher efficiency. Dual fuel partially premixed, compression ignition combustion, incorporating less reactive primary fuel mostly supplied by port injection and more reactive fuel directly injected into cylinder as chemical spark plug, is accepted to be highly effective for simultaneous improvement of fuel economy, smoke and NOx emissions as well (Lu et al., 2011; Thanapinyawanit and Lu, 2012). In addition, ethanol fuel could help to reduce soot emissions in a premixed mode (Chen et al., 2007).

Knock is characterized by amplitude pressure oscillations in the combustion chamber and can lead to engine failure or a total destruction through over-increased chemical energy and mechanical stress (Szwaia et al., 2007; Chiriac et al., 2006). It is found that knock is triggered by the spontaneous ignition of part of the unburned end-gas ahead of spark-ignited flame front (Borg and Alkidas, 2006; Brecq et al., 2003). In the best conditions approximately 60 % or higher diesel energy can be substituted with ethanol (Padala et al., 2013b; Sarjovaara et al., 2013). The increasing proportions of alternative fuels burned in premixed phase make dual-fuel engine combustion process more similar to the spark ignition engine (Abagnale et al., 2014). Critical aspects for dual-fuel engine are at full load, when high totally unburned hydro-carbon (HC) and carbon-monoxide (CO) emissions and heavy knocking usually occur, and the heavy knocking, caused by increased cylinder pressure rise rate, damages engine (Sarjovaara and Larmi, 2015; Goldsworthy, 2013). In normal diesel engine combustion, a single injection can be divided to a two stage injection to reduce early pressure rise rates. Sarjovaara et al. (2013) delve deeper into the effects of two stage injection on ethanol dual-fuel combustion. The study was conducted with a heavy-duty diesel engine with manifold ethanol injectors. They found that the diesel pilot injection is beneficial if above 50 % ethanol energy substitution is desired. By having a two-phase diesel injection, the PRR and maximum cylinder pressure decreased significantly and approximately 90 % ethanol energy percentages were achieved without suffering from too high cylinder pressures. A similar split-injection strategy was investigated by Sarjovaara and Larmi (2015) for increasing E85 rates in a dual-fuel heavy-duty diesel engine equipped with a common-rail injection system. They found that the issue of increasing E85 rates is not the pressure rise rate for all the cases, but in cases with the highest portions of E85, the limiting issue is the control system, which started to disable the pre-injection since the total amount of diesel reached a certain minimum level.

Extensive investigations have been carried out with numerical simulation methods to provide the information about the origin and the consequences of knocking combustion (D’errico et al., 2012; Lee et al., 2015b). There are roughly two different modeling strategies to simulate...