Artículo de Investigación / Research Paper

Heptane and Dodecane as surrogates of diesel fuel, a comparison with Computational Fluid Dynamics (CFD)

Heptano y Dodecano como sustitutos del combustible diesel, una comparación mediante Fluido-Dinámica Computacional (CFD)

A. L. Delgado-Mejia[1], L. C. Olmos-Villalba[2]

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Resumen

En este trabajo se ha efectuado un estudio comparativo entre dos combustibles de referencia como el n-heptano y el n-dodecano, ambos ampliamente utilizados como sustitutos del combustible diesel, en diversos estudios sobre inyección combustión y formación de emisiones contaminantes en motores diesel. Para ello se ha simulado la inyección evaporación y auto ignición de los combustibles mencionados utilizando un paquete de Fluido-Dinámica Computacional (CFD). Los resultados se han validado con información experimental proporcionada por los laboratorios SANDIA, llevados a cabo a diferentes condiciones operativas y con diferentes combustibles. La comparación se ha hecho en términos de parámetros típicos como la longitud de penetración, el lift-off de la llama y el retraso a la ignición.

Los resultados indican que hay una buena concordancia entre la simulación CFD y los datos experimentales, al comparar cada combustible sustituto. Sin embargo, al hacer

1 Magister en Ingeniería: Energética – Ingeniero Mecánico. Institución Universitaria Pascual Bravo. alvaro.delgado@pascualbravo.edu.co

2 Magister en Ingeniería: Energética – Ingeniero Mecánico. Institución Universitaria Pascual Bravo. luis.olmos@pascualbravo.edu.co

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la comparación con el diesel, el n-heptano fue el combustible sustituto que presentó un comportamiento más cercano al diesel, en términos del lift-Off y del retraso a la ignición.

Palabras clave: CFD, combustible sustituto, diésel, inyección, chorro.

Abstract

This paper has made a comparative study between two reference fuels such as n-heptane and n-dodecane, both widely used as surrogates for diesel fuel in several studies concerning on injection, combustion and emissions formation in CI engines. In order to achieve this it has been simulated the injection, evaporation and auto ignition of both fuels, using a Computational Fluid Dynamics (CFD) package. Results have been validated with experimental data provided by SANDIA laboratories, conducted at different operating conditions and with different fuels. The comparison is made in terms of typical parameters such as liquid penetration length, the flame lift-off and the ignition delay time.

Results indicated that there are a good concordance between CFD simulation and experimentation, when each surrogate fuel is compared. Nevertheless, when they were compared to D2 fuel, the n-heptane was the surrogate that best matched the D2 fuel behavior, in terms of Lift-Off length and ignition delay time.

Keywords: CFD solver, surrogate fuel, diesel fuel, injection, spray.

1. Introduction

Throughout the world, a large percentage of the cargo and passenger transport vehicles use diesel fuel as energy source. However, in most scientific works in which the diesel combustion and pollutant formation emissions are investigated, a reference fuel is used as surrogate for diesel fuel, some researchers work with n-heptane and others do with n-dodecane. In the first case, the n-heptane has a cetane number similar to diesel and the characteristics concerning to autoignition are best represented. In the other hand, n-dodecane is closer to the average number of carbon content of diesel fuel, therefore the mixing process and the mechanisms of formation of species tend to be more similar to those of commercial diesel, which results of great importance since the combustion in diesel engines is mixing controlled, as shown by studies conducted by You [1] and Westbrook [2] who performed various tests with n-alkanes ranging from the n-octane to n-hexadecane, in combustion processes with kinetic reaction schemes including 8157 reactions and 115 species. Although Sheen [3] made a review where compared different models for the oxidation of normal heptane. In general, the oxidi-

zation of large hydrocarbon fuels undergoes complex chemical processes, affecting the ignition and stabilization of the fuel spray and combustion [4]. From the point of view of modeling, a disadvantage of n-dodecane compared to n-heptane is the reduced availability of validated and relatively compact (for CFD) chemical mechanisms under CI engines relevant conditions [5]. Other authors have investigated different surrogates for diesel fuel; Pei et al [6] studied the behavior of n-dodecane saprays using the transported probability density function method for a numerical simulation in Fluent. Bhattacharjee et al [7] performed a similar study, but considering transient conditions and comparing n-heptane and n-dodecane. Meijer et al [8] focused on the degree to which the ambient thermochemical conditions can be replicated across different experimental facilities and developed some definitions corresponding to n-heptane spray, of global quantities including liquid and vapor penetration lengths, ignition delay, and lift-off length, and the extent to which these can be reproduced in different experimental facilities. Nevertheless, relatively few modeling studies have been reported for the n-dodecane spray flames. Ayyapureddi [5] explored sensitivities of the spray model results to variations in the spray entries, for one of the experiments carried out in the ECN Spray A flames. Som et al. [9] compared computed and measured ignition delays and lift-off lengths over a range of initial temperatures using a well-stirred reactor for combustion model in a Reynolds-averaged formulation, with two different ambient gas densities (15% O^2, 22.8 kg/m^3). Pairy et al [10] examined the effect of fuel temperature on the spray characteristics of n-dodecane in a novel continuous flow chamber.

The purpose of this work is to compare the behavior of two reference fuels, n-heptane and n-dodecane, both of them widely used as surrogates of diesel fuel, during the process of injection, evaporation, mixing and ignition, at similar conditions to those at which typically operates compression engines.

2. Materials and Methods

2.1. The CFD code

In this work, the simulations have been performed by means of OpenFoam, which is an open source CFD software package created to deal with complex fluid flows, involving chemical reactions, turbulence and heat transfer. It was written

in C++ and it is based in the finite volume method to solve the systems of partial differential equations, on any 3D unstructured mesh of polyhedral cells. For this study, the simulation was based on the AachenBomb case that is computed with the sprayFoam solver. A major description of this solver can be found in the User Guide [10] of the software and in the project work made by Arshad [11]

2.2. Model formulation

Mixture formation and combustion process in diesel engines are simultaneous processes with a strong dependence between each other, being the fuel injection, liquid atomization and evaporation, the energy, mass and momentum exchange, the most influencing. At the same time chemical reactions take place allowing the auto ignition of fuel, the burnout of the premixed phase and the diffusion combustion.

Considering that the numerical simulation of fuel injection and mixture formation is a combination of the Eulerian approach for the gas-phase and the Lagrangian description for the droplet-phase, the spray atomization and break up, droplet collision and evaporation, turbulence, ignition and combustion must be implemented in the simulation code.

The spray model employed in this work was the Kelvin-Helmholtz-Rayleigh-Taylor (KH-RT) model, proposed by Reitz [13, 14, 15], which was developed originally for reference hydrocarbons, but it can be extended to other fuels, provided the physical properties are well defined [16]. The model is based on the assumption that the growing of the instabilities of Kelvin – Helmoltz over the surface of a cylindrical liquid jet that penetrates into a stationary gas, is linear. This model has been widely applied in several works, in order to simulate primary as well as secondary break up [17].

A precise determination of ignition delay time depends of the criterion used, fuel consumption, formation of CO, formation of OH, increase of pressure in a constant volume vessel, increase of temperature in an adiabatic vessel, etc. [18]. The auto ignition model adopted in this work was the so called Shell Model, developed originally by Halstead et al [19] in order to predict knock in spark ignition engines, but later adjusted and applied to modeling diesel ignition, as described in [20, 21]. The main characteristic of the Shell model is that it involves eight reaction steps between five species, representing a virtual mechanism that attempts to reflect the actual ignition behavior of hydrocarbon-air mixtures, including multistage ignition and cool flames.

The turbulence model chosen in this work was the RNG k–ε model, modified for considering the effect of compressibility and the interaction with the spray, because of its simplicity and lower CPU time consumption.

The combustion model is based in the concept of partially stirred reactor (PaSR), which has been developed and adapted for the OpenFoam code by Nordin [22]. The reaction scheme used in the simulations was one of the reduced type, including 15 species (C_7H_{16}, O_2, CO_2, N_2, H_2O, CO, O, OH, H, H_2, HO_2, H_2O_2, N, NO y C) and 39 reactions, as can be seen in figure 1. The entire set of models and submodels for the simulation are listed in table 1.

TABLE 1. MODELS AND SUBMODELS USED IN THE SIMULATION [11]

Phenomena	Model
Atomization	blobSheetAtomization
Break Up	Reitz KHRT
Drag	standardDragModel
Evaporation	standardEvaporationModel
Heat Transfer	RanzMarshall
Turbulence	k-e
Ignition	Shell
Combustion	PaSR (Partially stirred Reactor)

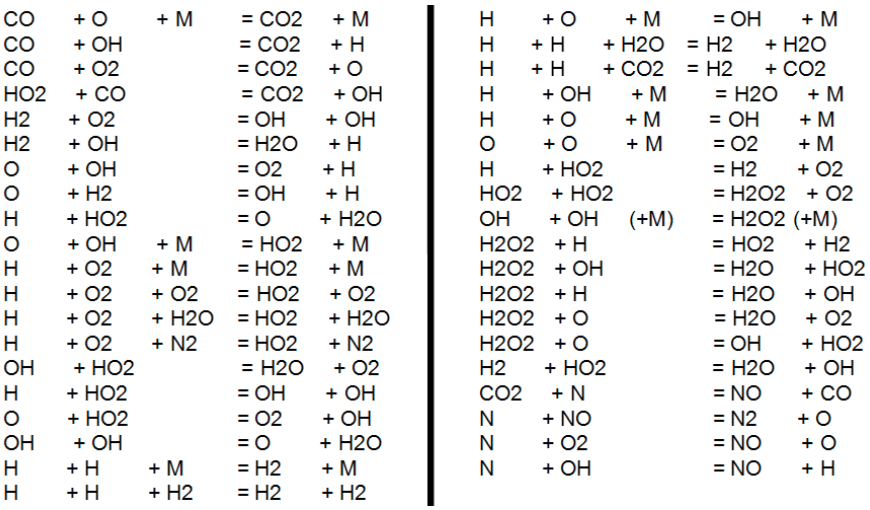

FIGURE 1. SCHEME OF CHEMICAL REACTIONS USED FOR THE SIMULATION IN REACTING CONDITIONS [11]

2.3. The experiments

Recently, Sandia National laboratories [23], by means of the Engine Combustion Network (ECN) conducted a series of high fidelity measurements in an optically accessible, constant volume combustion vessel, with cubic geometry, concerning with the spray and combustion characteristics of several fuels, including n-heptano, n-dodecane and diesel #2, for a wide range of combustion vessel temperature (450 K – 1300 K), vessel density (3 kg/m^3 – 60 kg/m^3), nozzle diameter (0.05 – 0.5 mm), oxygen concentration (0% - 21%) trying to simulate different levels of EGR and injection pressure (40 MPa – 200 MPa). The injection system is representative of the modern common-rail injection systems. Pickett [24] presents a broad explanation of the experiments. Results obtained by some authors, from earlier modeling studies of the ECN sprays have been presented and discussed at the ECN workshops, and several modeling studies have been published in recent years.[23]

2.4. Computational model

The simulation was carried out in a cubic shaped combustion chamber, Fig. 2, with the same dimensions of the Sandia constant volume vessel [22], and validated with the data available on its website, including reacting and non-reacting sprays in a constant volume chamber, in like diesel engine conditions and with several fuels.

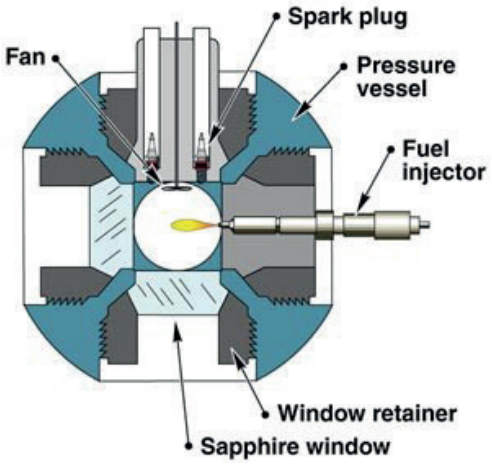

FIGURE 2. SCHEMATIC CROSS - SECTION VIEW OF THE EXPERIMENTAL COMBUSTION CHAMBER [23]

The corresponding mesh model of the vessel used for the study (Figure 3) consisted of a 108 mm side cubic box, with approximately 200000 computational cells. This mesh density resulted from a previous sensitivity study of grid dependence, in which five mesh grids with 100000 cells, 200000 cells, 225000 cells, 250000 cells and 300000 cells were simulated in conditions of reacting and non-reacting diesel spray. The analysis allowed to conclude that from 200000 cells, the results was practically the same.

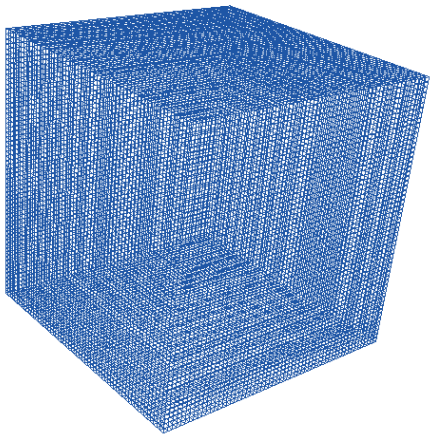

FIGURE 3. MESH GRID OF THE VESSEL

The operative conditions for the simulations performed are listed in Table 2, and the properties of the fuels are listed in table 3.

TABLE 2. Conditions for the simulations

Ambient gas oxygen concentration	21	%
Ambient gas temperature	800 → 1200	K
Ambient gas density	14.8	kg/m^3
Injector Orifice diameter	0.1	mm
Injection pressure difference	150	MPa
Fuel type	n-heptane, n-dodecane	
Fuel temperature	373	K

The study was made in terms of the typical parameters of liquid sprays, such as length penetration, lift-off length and ignition delay time.

TABLE 3. FUEL PROPERTIES FOR BOTH SURROGATES AND D2 FUELS [11,23]

Fuel property	n-Heptane	n-Dodecane	D2
Chemical formula	C_7H_{16}	$C_{12}H_{26}$	33.8% aromatics 65%parafinics 1.1% alefines
Density (kg/m³)	688	750	843
Molecular weight (kg/kmol)	100.2	170.3	---
Viscosity (mPa s)	0.386	1.34	1.98
Vapor pressure (Pa)	5.33	18	---
Flash point (K)	269.1	356	346
Autoignition temperature (K)	496	478	---
Boiling point (K)	372	487	310
Cetane number	56	47	87

3. Results and Discussion

Liquid penetration is defined as the axial location spanning about of 97% of the injected mass at that instant of time. For the non-reacting conditions, figure 4 shows simulated and measured liquid spray penetration as a function of time after the start of injection (ASOI) at a combustion chamber temperature of 900K. Initially the spray penetration increases strongly with time and then stabilizes at a constant value near to 10 mm. The reason for this trend is because beyond this axial distance, liquid fuel has evaporated and only exists the gas phase. There is no a strong evidence that allow to conclude that any of surrogates be more similar to D2 fuel performance, because the penetration profiles are almost the same. In the early stages of the process (0.1 ms), CFD Simulation captures the liquid and global spray characteristics better.

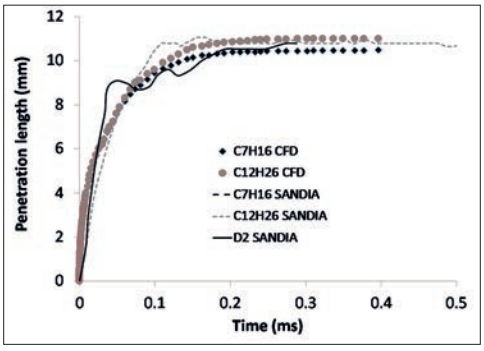

FIGURE 4. LIQUID SPRAY LENGTH (mm) AS A FUNCTION OF TIME

Among several criteria used to measure the ignition delay time of sprays injected into high pressure and high temperature combustion chamber, the most common are the pressure rise, the temperature rise and the burnt fuel associated to ignition. Figure 5 plots the CFD results for the pressure rise, compared with the corresponding experimental measurements, for the case depicted in table 2, for n-heptane fuel. After the injection there is a slight fall in the pressure and temperature inside the vessel, due mainly to the evaporation, but in a short interval of time, in the order of 1 ms, occurs a sudden increase due to the chemical reactions and allowing the auto ignition to take place. It is usual to assume that when such increase is positive, near to 10 kPa, then it can be established that ignition has occurred. For those conditions, the ignition delay reported by Sandia was 0.65 ms and the value obtained by the CFD simulation was near to 0.92 ms. CFD simulation matches fairy well the experimental delay time reported in the Sandia experiments for the same conditions.

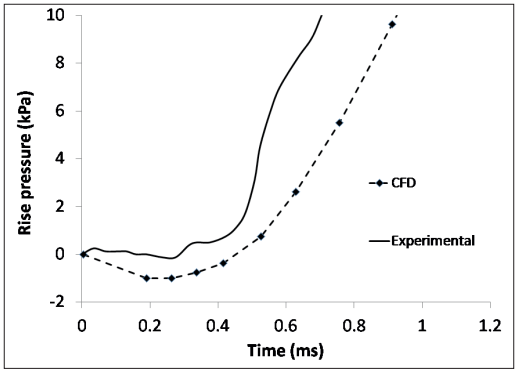

FIGURE 5. PRESSURE RISE FOR 800 K AND 21% O2

Figure 6 plots measured and predicted ignition delay vs temperature (ASOI) at a combustion chamber temperature of 900 K. Although the behavior is the same than lift – off length, it can be observed that n-heptane matches better the D2 fuel in the entire range of temperatures, but at temperatures higher than 1100 K the n-dodecane tends to be more similar, in the case of simulation results. For the experimental data, the n-heptane was the fuel closer to the reference fuel, almost in every temperature, which can be explained by the similar cetane number between them.

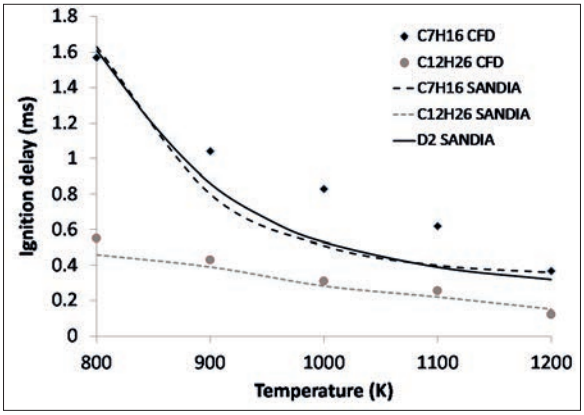

FIGURE 6. IGNITION DELAY TIME (ms) AS A FUNCTION OF TEMPERATURE, FOR 21% O2

The lift-off can be defined as the axial distance from injector to the zone of high-temperature reaction, and usually it is measured by means of OH concentration, because it exists as an equilibrium product in regions of high temperature and results from chemical reactions in near-stoichiometric, high-heat-release regions [25]. The lift-off length results, for the conditions simulated, reported are in a good agreement with the experimental results. Figure 7 presents the comparison between surrogates and D2 fuel; all of them exhibit the same trend, e.i the lift-off length decreases with temperature, because of high temperatures improve auto ignition and accelerate the kinetics of OH reaction [26]. In this case, both, CFD simulation and experimentation, demonstrate that n-heptane has the best matching with D2 fuel at high and low temperatures. Figure 8 compares the results obtained by the CFD simulation for OH radical concentration when the combustion chamber temperature was 1000 K, the oxygen concentration 21% and the injection pressure of 1500 bar, which gives the OH concentration every 200 μs; from this colormap can be determined a lift - off approximately of 20 mm. For the same conditions, the ignition delay reported by Sandia was 16.5 mm. The image was obtained by means of OH chimioluminiscence [23], for conditions of 1000 K, 21% O2, 150 MPa of injection, 0.1 mm nozzle diameter and n-heptane as fuel.

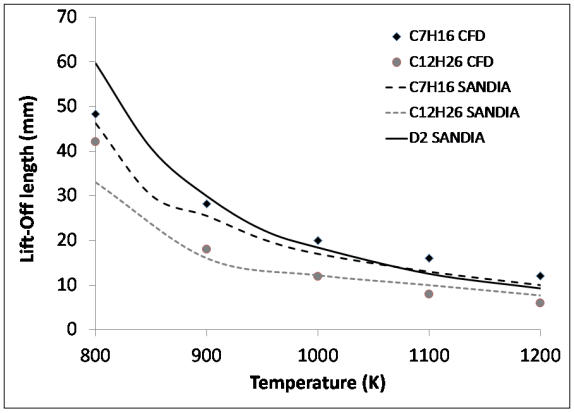

FIGURE 7. FLAME LIFT-OFF LENGTH (mm) AS A FUNCTION OF TEMPERATURE, FOR 21% O2

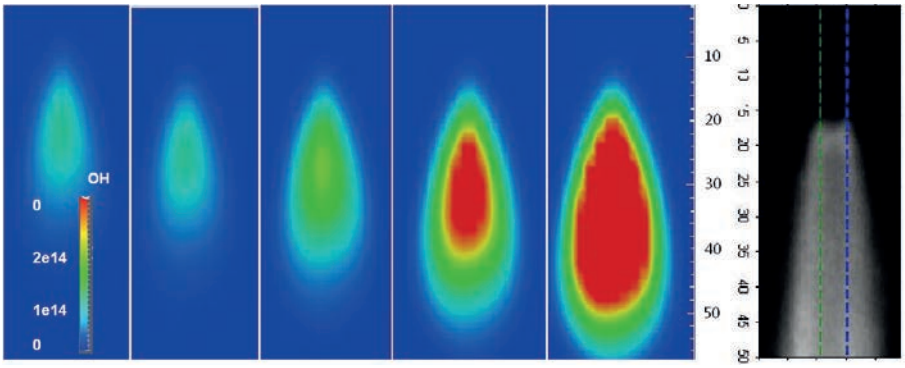

FIGURE 8. CFD APROXIMATION OF FLAME LIFT-OFF, BASED IN OH CONCENTRATION (VOLUMETRIC FRACTION) AND MEASURED OH BY MEANS OF CHIMIOLUMINISCENCE.

4. Concluding remarks

A comparison between two surrogate fuels (n-heptane and n-dodecane) for diesel fuel have been performed by means of CFD simulations using OpenFoam, varying temperature inside combustion chamber and for other conditions similar to those in which operates CI engines. These results were validated with experimental data published by Sandia National Laboratories [23].

- The simulations were able to reproduce the liquid fuel distribution very well, which is consistent with results presented above for reacting and non-reacting conditions.

- The liquid spray penetration profiles were practically the same for all the fuels considered, and there is no evidence to conclude about which surrogate matches properly the D2 fuel.
- Ignition delay time of n-heptane was the closest to D2 fuel, which can be expected taking in account the fact that both fuels have similar cetane number, one of the most influencing parameter on ignition of hydrocarbons fuel. The method of determining ignition delay by means of pressure rise resulted a good choice.
- Flame lift – Off length allowed to conclude that, for the conditions analyzed in this work, n-heptane is the best surrogate for diesel fuel, in terms of the results of CFD simulation and in terms of experimental data.
- Although more simulations must be carried out, the convenience of using CFD packages is evident. As a future work, it is recommended the exploration of more detailed turbulence model in the study of sprays.

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