López Sánchez, JJ.; Novella Rosa, R.; García Martínez, A.; Winklinger, JF. (2011). Investigation of the ignition and combustion processes of a dual-fuel spray under diesel-like conditions using computational fluid dynamics (CFD) modeling. Mathematical and Computer Modelling. 57:1897-1906. doi:10.1016/j.mcm.2011.12.030.

Investigation of the Ignition and Combustion Processes of a Dual Fuel Spray under Diesel-like Conditions using CFD Modeling

J.J. López, R. Novella*, A. García, J.F. Winklinger

CMT-Motores Térmicos, Universidad Politécnica de Valencia, Camino de Vera s/n, 46022 Valencia, Spain

Abstract

Recent research activities in the field of Diesel engines have shown the potential to reduce pollutant emissions and improve thermal efficiency by controlling fuel reactivity. However, understanding the impact of blending fuels with different physical and especially chemical properties on diesel-like spray mixing and combustion processes is still a challenge. Since the experimental techniques are still far from providing detailed temporal and spatial information about local spray conditions, CFD modeling tools arise as the key source of information to investigate the characteristics of these dual fuel sprays. In this frame, the present research focuses on modeling a dual fuel spray in diesel-like conditions, comparing different gasoline and diesel blends in terms of ignition characteristics and flame structure. The results confirm the suitability of the state of the art computational CFD modeling tools for reproducing the complex phenomena associated to dual fuel sprays. Moreover, the important benefits provided by dual fuel blends, considering the expected reduction in pollutant emissions as a consequence of the differences observed in terms of flame structure, are confirmed.

Keywords: CFD Modeling, Dual Fuel, Diesel Combustion, Mixing controlled Combustion, Spray Ignition

*Corresponding author

Email address: rinoro@mot.upv.es (R. Novella)

1. Introduction

Throughout the last decades, the most widely-used power-units in road vehicles have been the gasoline (or spark-ignition, SI) and the diesel (or compression ignition, CI) internal combustion engines. However, it is worthy to note that diesel engines use oil-based fuel 25-40% more efficiently than gasoline engines. Therefore, they provide a promising means of lowering fuel consumption (and CO_2 emissions) until a more sustainable solution is found [1]. While the diesel engine has been used in road transport throughout the world almost exclusively in heavy-duty applications because of its outstanding fuel economy, durability, reliability and performance [2], it has not been considered as a suitable power train for light-duty vehicles and for passenger cars due to excessive noise and its less "fun-to-drive" characteristics. Recently, this scenario has changed and the development of diesel engine technologies is the main responsible for the increment in the share of vehicles equipped with a diesel engine in the European market, from around 12% in 1995 to 50% in 2005 [3].

Nevertheless, as a main drawback, the diesel engine is also well known as a significant source of pollutant emissions, including nitrogen oxides, unburned hydrocarbons, carbon monoxide and particulate matter (mainly soot). Stringent regulations are being introduced around the world to limit its environmental impact. Specifically, conventional fuels used in current diesel engines have cetane numbers (CN) greater than 40 and auto-ignite very quickly after the start of injection in the cylinder. Particularly at high loads, fuel continues to be injected after the combustion has started and this leads to high NO_x and soot formation. Thus, if the mixing is accelerated or if the chemical reactions are slowed down, auto-ignition can be made to occur after the fuel is injected, achieving a better mixing process, and soot levels can be reduced. Consequently, on this concern, it would be desirable to have a fully premixed combustion. NO_x levels can be reduced by reducing combustion temperature by either running lean, premixed or using EGR (Exhaust Gas Recirculation). In fact, an outstanding technology is currently used in advanced diesel engines, making them expensive and complicated, to counteract the high ignitability of the diesel fuel in order to promote premixed combustion. Even then, with conventional diesel fuels, low NO_x and low soot with partially premixed CI combustion is possible only at low loads. Modern engines still require complex after-treatment systems to further reduce NO_x and particulates, making the power train even more complicated and expen-

sive.
A new way to overcome this situation is to change and control the reactivity of the fuel. Thus, two fuels with different reactivity characteristics (for instance diesel and gasoline fuels) can be blended (in a convenient proportion) and injected in the cylinder with the same fuel injection system. Concerning this dual-fuel framework, several works [4, 5, 6, 7, 8, 9, 10, 11, 12, 13] have shown that CI engines can be run on fuels in the gasoline auto-ignition range if appropriate injection timings and strategies are used. Moreover, the higher resistance to auto-ignition associated with such fuels allows more time for the fuel to mix with the air before combustion and greatly facilitates low NO_x and low soot operation, showing the dual-fuel potential.
In spite of the existence of the commented engine results, there is a lack of comprehensive experimental studies in this field. Basically due to the impossibility to use experimental techniques in diesel-like conditions capable to well separate the effects of diesel and/or gasoline in the main local spray characteristics. On the other side, computing is now truly on a par with experiments and theory as a research tool to produce multi-scale information that is not available by using any other technique [14]. In the particular case of combustion in diesel-like conditions, Reitz and Rutland [15] point out how additional aspects should be considered since combustion characteristics are greatly influenced by the details of the fuel preparation process [16] and the local distribution of the fuel in the combustion chamber which is, in turn, controlled by fluid mechanics. Fuel injection introduces the complexity of describing the physics of sprays [17, 18], defined as vaporizing two-phase flows that vary spatially and temporally from very dense to fairly diluted conditions. Thus, different submodels have been developed for processes occurring on time and length scales that are too small to be resolved, such as atomization, breakup, droplet drag, vaporization, coalescence, turbulence, dispersion, spray-wall interaction and turbulent combustion.
From the previous paragraphs it can be deduced that, on the one hand, the use of dual fuel in CI engines is a promising way to achieve a clean and efficient engine. On the other hand, multidimensional CFD calculations seem to be a proper tool to comprehend the specific changes introduced in the spray combustion characteristics due to the use of the dual fuel concept. Therefore, the main objective of the present paper is focused on evaluating the effects of diesel/gasoline blends on mixing, autoignition and flame structure in diesel-like conditions by means of CFD calculations. After this introduction, the methodology and tools employed for this work are described. Next, the ef-

fects of dual fuel blends on flame ignition and combustion are discussed, and finally, the main outcomes of the work are presented.

2. Methodology

The general methodology followed along this work starts with an adjustment of model parameters and the subsequent validation of the spray modeling and turbulent mixing, explained more in detail in subsection 3.4. Moreover, in order to reduce the computational effort, a chemistry model with a reduced kinetic mechanism was adopted and validated to justify its use considering the requirements of this investigation. The model and its validation are described in subsection 3.5.
Finally, this validated setup was used for the current investigation which compares the spray ignition and combustion processes of two different diesel-gasoline dual fuel blends to pure diesel fuel.
Actually, in this work diesel and gasoline were modeled using primary reference fuels (PRF). Iso-octane was used to represent the physical and chemical properties of gasoline in both liquid and gas phase. On the one hand the properties of tetradecane were adopted to model diesel in its liquid state. On the other hand, n-heptane was used to describe the properties of diesel in the gas phase. This approach of modeling the physical and chemical properties of diesel yields reasonable results as shown in [19]. Moreover, studies (e.g. [20]) have shown that iso-octane and n-heptane are two well suited PRFs to represent gasoline and diesel combustion, respectively. Also the combined adoption of these two primary reference fuels for blends of diesel and gasoline provides good agreement [21].
The three modeled cases are named after the respective mass fraction of diesel, "100%" for the pure diesel fuel case, "80%" and "60%" for the case with 80% diesel, 20% gasoline and the case with 60% diesel, 40% gasoline, respectively. The fuel blends were injected as a single spray at a temperature of 360K in a constant volume vessel with adiabatic walls. Hereby, spray-spray and spray-wall interaction as well as the modeling of a moving piston were avoided. The ambient conditions were set according to the Spray A operating conditions [22], i.e. an ambient temperature of 900K and an ambient pressure of 60bar, being representative for current and future diesel engine operating conditions. However, the oxygen mass fraction was kept at 22.8% to simulate conditions without exhaust gas recirculation (EGR). Moreover, the experimental results of the inert Spray A case were used in the validation

process.

3. Computational Models and numerical Setup

The CFD calculations were carried out with the open source CFD package OpenFOAM® [23] in its version 1.6. In this particular investigation the dieselFoam solver, which is able to simulate fuel spray and combustion, was selected. This code solves the gas phase in an Eulerian framework, and a discrete droplet method (DDM) approach [24] is applied for modeling the liquid fuel spray. In doing so, parcels, representing a class of identical, non-interacting spray droplets, are tracked through the physical space in a Lagrangian way, taking into account the mass, momentum and energy exchange with the gas phase.
Furthermore, several submodels are applied by the dieselFoam solver to model the physics of the fuel spray, and the adopted turbulence model accounts for the turbulent mixing of fuel and air. These adopted models are briefly described in the following sections. Finally, the combustion of the fuel-air mixture is modeled by means of the Chalmers' Partially Stirred Reactor (PaSR) combustion model [25].

3.1. Turbulence Model

The Reynolds Averaged Navier Stokes (RANS) approach is used in the dieselFoam code to model turbulent flow. Here in particular, the standard k-ε model [26], a widely used two-equation turbulence model, was used in this work. This model solves for the turbulent kinetic energy k and the isotropic turbulent dissipation rate ε. During the spray and mixing validation process the model parameter C_1 was changed to 1.52 for best agreement of modeling and experimental results concerning liquid and spray penetration, as shown in Fig. 1. A necessary tuning of this parameter of the k-ε model for better approximation of axisymmetric jets is known, and the same value is suggested in [27].

3.2. Spray Submodels

The DDM approach requires the adoption of submodels in order to describe the spray atomization, breakup, dispersion, drag and evaporation. The Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) hybrid model [28] was used for atomization and breakup modeling and the Ranz-Marshall model was applied for droplet evaporation [29]. Initially, the same submodel setup as described

in [30] was adopted.
However, in order to better represent the atomization and breakup processes close to the injector outlet and, in addition, to better fit liquid and vapor penetration at the beginning of injection, some modifications were made on the submodels. Parcels within the intact core of the liquid fuel jet are only affected by atomization but neither by drag nor by evaporation. The validation showed that simulation results best approximate the experimental data for a liquid core length equal to seven times the equivalent diameter. This model parameter connecting the length of the liquid core with the equivalent diameter is within the range stated in [31]. Thus the liquid core length is in the order of five millimeters. Droplets outside this core length are subjected to breakup, drag and evaporation. A similar modeling approach is presented in [32].

3.3. Computational Grid

In this work all calculations were performed on the same model domain consisting of a 2D axisymmetric structured mesh. This mesh represents a cylindrical combustion vessel of 54mm in radius and 108mm in length. Because of the high sensitivity of the Lagrangian submodels to the cell size in connection with the time step size, the cell size was determined in a parametric validation process. Finally, it was set to 0.5mm in axial direction and 0.25mm in radial direction.

3.4. Spray and turbulent Mixing Validation

As already mentioned above, an extensive validation process was carried out before the current investigation to assure the proper application of the turbulence model and spray submodels in interaction with the computational grid and time step size (Δt = 0.1μs).
At the beginning, the experimental data of the inert Spray A case from the Engine Combustion Network (ECN) [22] was chosen as benchmark to adjust the CFD model setup. This means that all preliminary calculations were performed under inert conditions avoiding the influence of combustion on spray development and mixing.

The calculation results of two of the main parameters of liquid sprays, the liquid length and the vapor penetration, are compared in Fig. 1 to the experimental data. Moreover, the modeling results of the radial distribution of fuel mass fraction at two different axial positions are compared in Fig. 2 and Fig. 3 to the experimentally obtained distribution. As a conclusion of

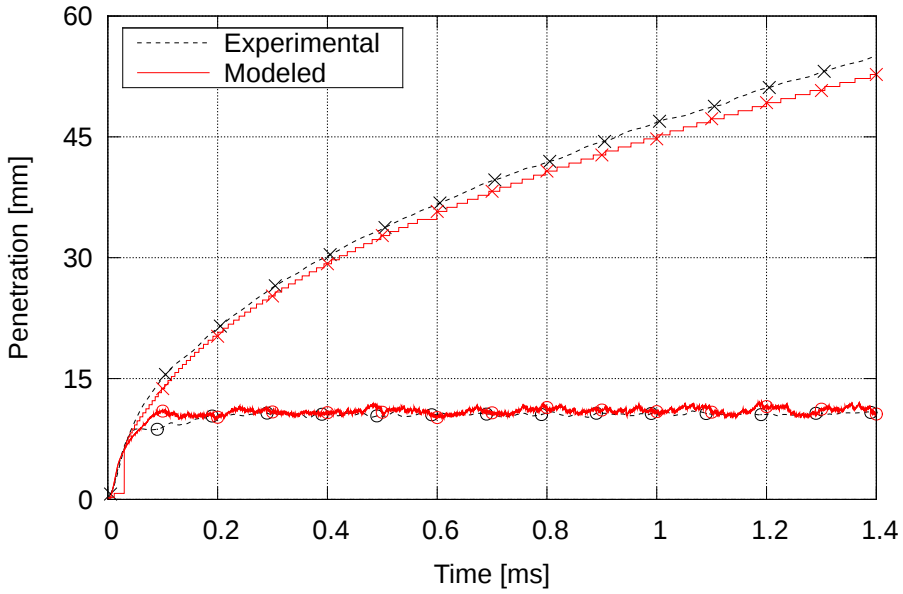

Figure 1: Model validation. Modeled vs. experimental liquid (circle) and vapor (cross) penetration

this preliminary validation process, it can be stated that the obtained CFD results show reasonable agreement with the experimental data. Hence, the setup is considered to be suitable for the further investigation.

3.5. Chemistry Model

In order to reduce the computational effort, a chemistry model with reduced a kinetic mechanism was adopted. The model used was published by Jerzembeck et al. [33] and includes 203 species and 1071 reactions. It was derived from the Lawrence Livermore detailed n-heptane and iso-octane mechanism.

In Fig. 4 a comparison of the reduced Jerzembeck mechanism and a detailed chemistry model from Curran et al. [34] with experimental data is shown. This validation was done to ensure the mechanism's applicability for modeling the auto-ignition and flame propagation characteristics of both fuels in this work. The reduced mechanism fits well the results obtained with the detailed mechanism which includes more species and reactions. Furthermore, the correlation with experiments can be considered sufficiently accurate.

Moreover, another important fact can be seen in this figure when comparing

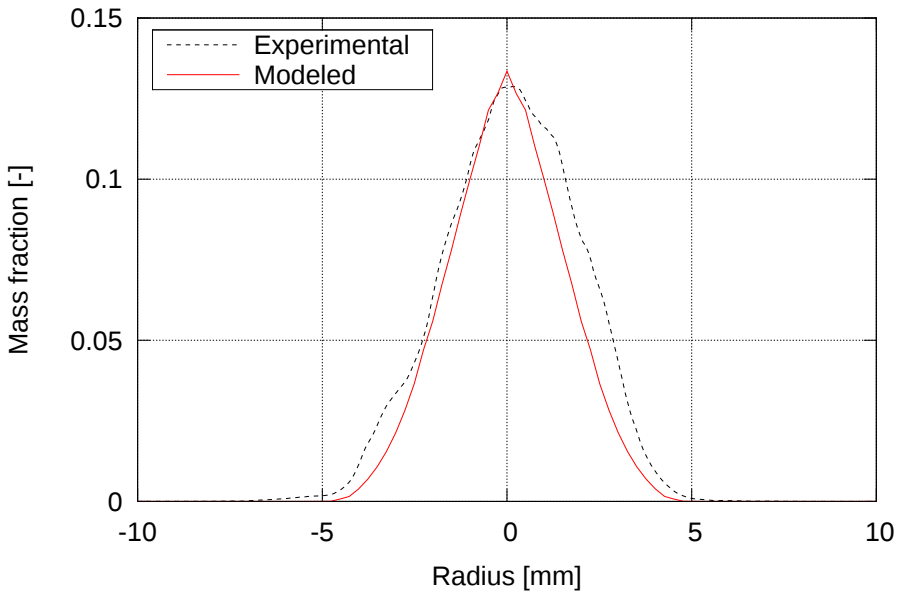

Figure 2: Model validation. Radial fuel distribution profile at 25mm from injector tip, 1.4ms after start of injection

the two fuels. Especially in the low temperature range, iso-octane possesses significant higher ignition delay than n-heptane.

4. Results

The main objective of this work was to determine the influence of modified fuel reactivity on the spray ignition and combustion processes. Therefore, the results shown in this section are chosen in order to identify the differences found in this investigation. The first subsection focuses on the auto-ignition process and the start of combustion. The impact on the flame structure is shown in the second subsection of this section.

4.1. Auto-ignition Analysis

Fig. 5 represents the temporal evolution of the maximum temperature in the vessel. All fuel blends reach the same steady-state maximum temperature value since diesel and gasoline possess similar heating values. However, temporal differences in the temperature rise can be observed for the three different fuel blends. An important parameter for the auto-ignition analysis

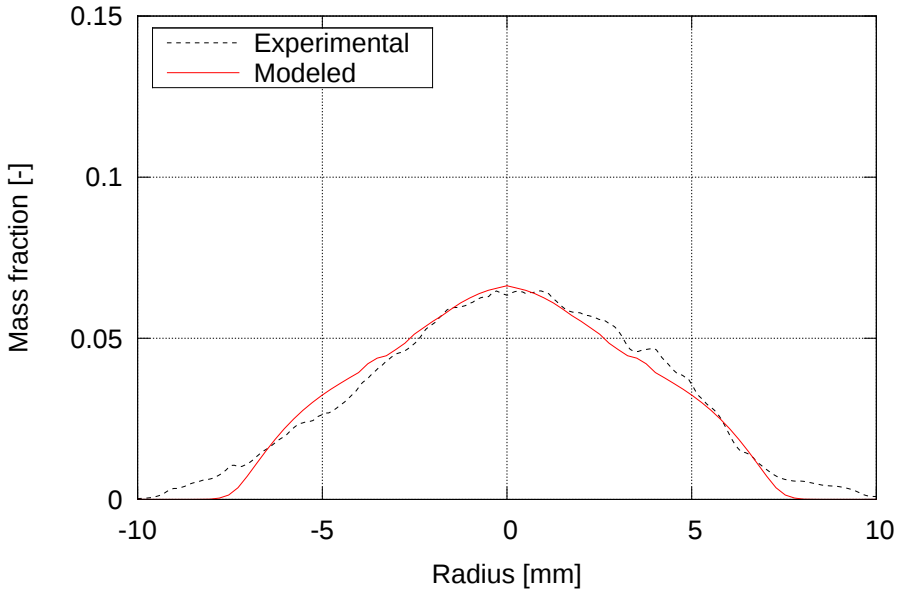

Figure 3: Model validation. Radial fuel distribution profile at 47mm from injector tip, 1.4ms after start of injection

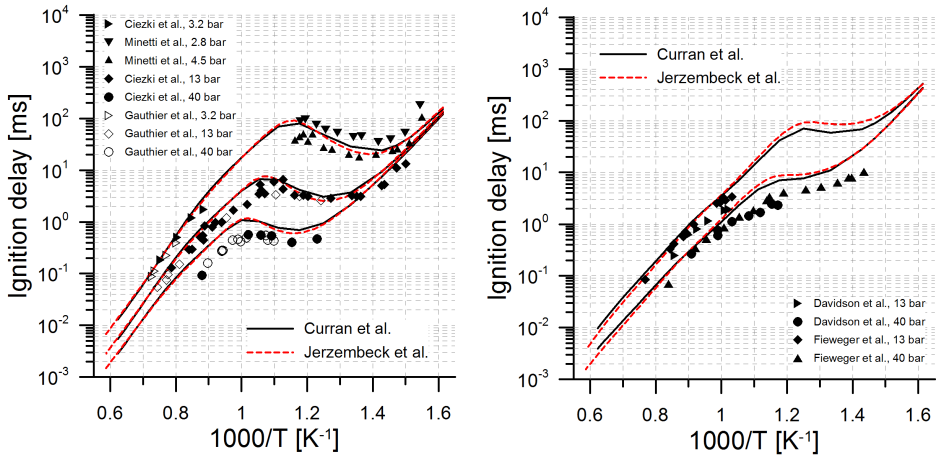

Figure 4: Validation of chemistry model. n-heptane (left) and iso-octane (right)

is the ignition delay which is defined as the time between start of injection and the onset of combustion. Specifically, as in a previous research [30], an increase of 400K of the maximum temperature over the ambient temperature indicates the ignition delay. This time gap is represented for each fuel blend

in Fig. 6, where pure diesel fuel shows the shortest ignition delay. A progressive increase of ignition delay is observed with increasing gasoline proportion in the blend. This outcome goes along with the difference in ignition delay of pure n-heptane and iso-octane. Moreover, these results confirm the potential of fuel blending to control the reactivity of the spray.

Furthermore, it is interesting to look at the temporal evolution of pressure

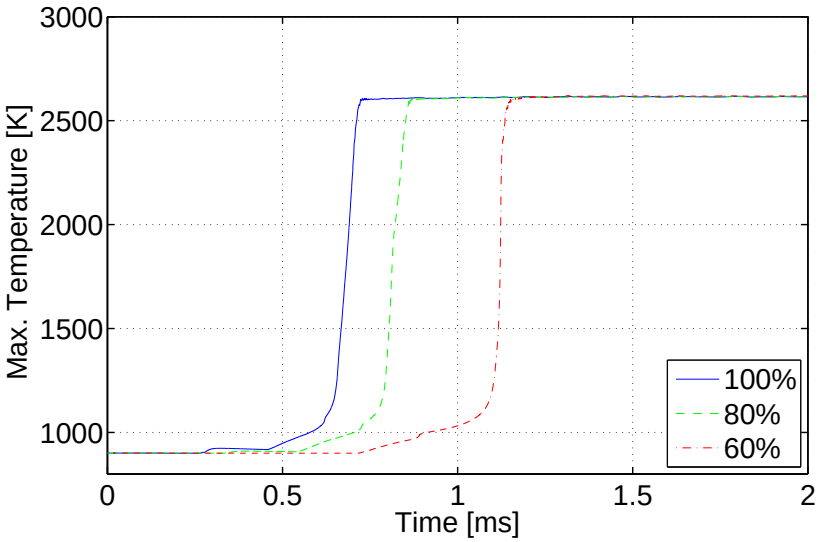

Figure 5: Ignition delay analysis. Temporal evolution of maximum temperature

change in the combustion vessel (defined as $\Delta p = p(t)\text{-}p_{initial}$), since this parameter is also affected by a modification of the fuel properties. A higher proportion of gasoline in the injected fuel mixture causes a slightly smoother rise of pressure as depicted in Fig. 7. So not only the reactions related to the onset of combustion, but also those active later on in the combustion process are slowed down by introducing fuel with lower reactivity. Despite the higher amount of fuel available for combustion at advanced injection time in case "60%", the reduced reactivity causes a decreased rate of pressure change compared to case "100%".

In the following, a sequence of CFD results show the spatial distribution of the fuel spray at the start of combustion (SOC), 0.02ms and 0.05ms after SOC. The colors in these images represent the equivalence ratio ϕ in a plane through the spray axis. Additionally, in a second layer the temperature

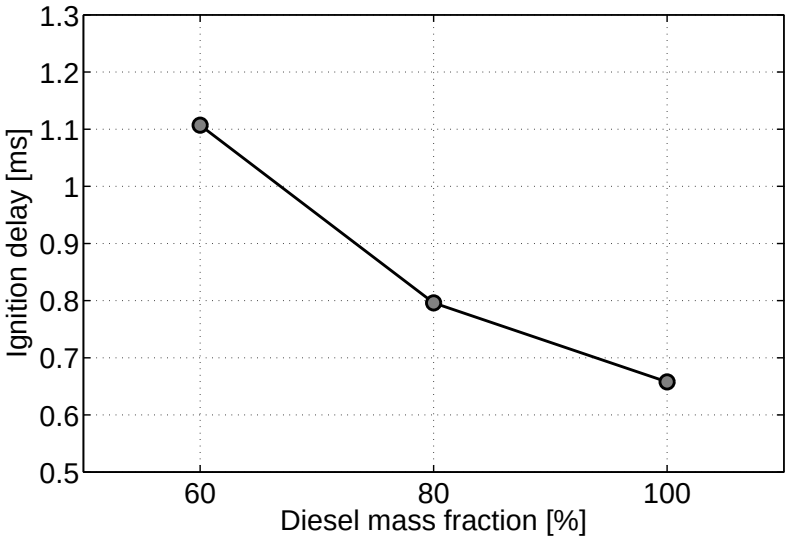

Figure 6: Effect of the fuel blend proportion on ignition delay

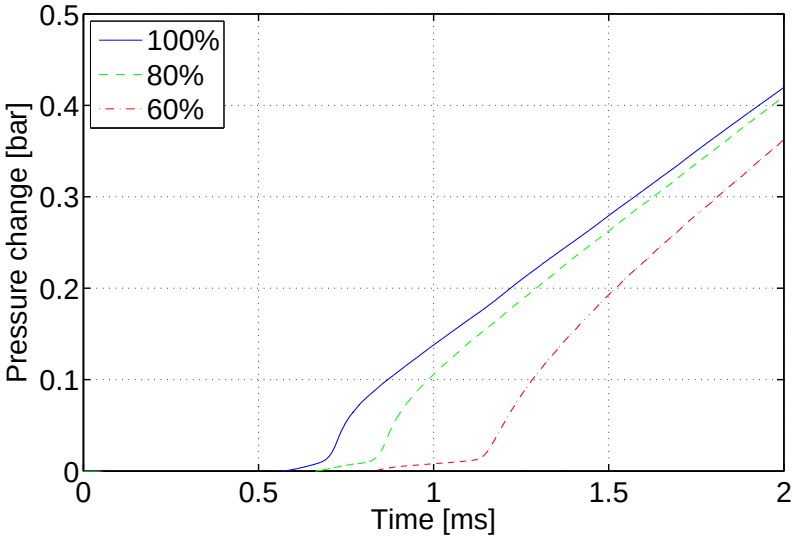

Figure 7: Comparison of the temporal evolution of pressure change

contours are plotted in regions where the temperature exceeds the ambient temperature by more than 400K, thus higher than 1300K. The three black lines mark equivalence ratios of 2, 1 (stoichiometric equivalence ratio) and 0.2, going from the rich center of the spray to the lean boundary of the spray. Moreover, the images are horizontally divided into two halves, the top one showing the pure diesel fuel spray and the bottom half a spray with a fuel blend of 60% diesel and 40% gasoline. The 60/40 blend was selected to be presented here because it shows larger differences compared to the pure diesel fuel than the 80/20 blend. The times depicted in each half of an image indicate the time after start of injection (SOI). In the top image the instant at start of combustion (SOC) of the pure diesel and the diesel-gasoline blend is depicted. Since the diverse fuel blends possess different ignition delays, the stated times do not coincide.

Additionally to the differences in terms of ignition delay, also a spatial difference on the combustion propagation can be observed. Reacting zones, identified by temperatures over 1300K, are different for varied diesel-gasoline proportions. Especially in the bottom image of Fig. 8, 0.05ms after the combustion onset, the differing shapes of the reacting zones as well as the different levels of equivalence ratios where combustion occurs can be detected. The last fact gets even clearer when plotting temperature versus equivalence ratio for both, diesel fuel and the 60/40 diesel-gasoline blend, as shown in Fig. 9 for the same instants again. The ignition process of the pure diesel fuel spray starts at equivalence ratio values between 2.5 and 3, whereas the 60/40 diesel-gasoline blend ignites at an equivalence ratio of approximately 1.5. Furthermore, as the combustion advances, the highest temperatures tend to appear at zones with stoichiometric mixture.
In summary, the results evidence how controlled fuel reactivity, by adjusting blend proportions, introduces temporal and spatial changes in the auto-ignition process. The onset of combustion is shifted toward zones with lower equivalence ratio.

4.2. Flame Structure Analysis

In addition to the auto-ignition process described in the previous subsection, the structure of the lifted turbulent diffusion flame associated to the fuel spray combustion is investigated in this subsection.
A key parameter of such flames is the lift-off length (LOL), which is a widely studied property in the field of spray combustion [35, 36]. This characteristic distance is defined as the shortest distance between the injector nozzle

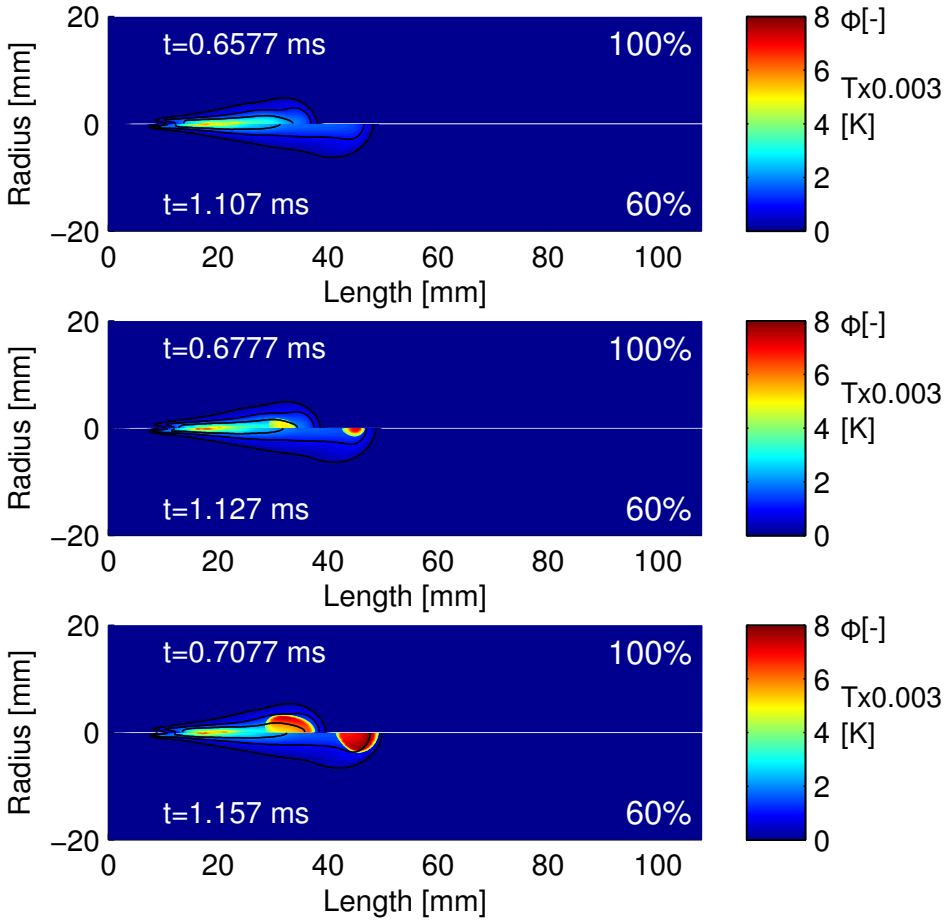

Figure 8: Comparison of the spatial distribution of spray and ignition sites of pure diesel (top half) and 60/40 diesel-gasoline blend (bottom half). Top image: at start of combustion (SOC), middle image: 0.02ms after SOC, bottom image: 0.05ms after SOC

tip and the most upstream location of combustion in the fuel spray. Experiments [37] have proven that LOL is a time varying property since combustion progresses against the spray flow toward the injector nozzle until it reaches a stabilized value. State of the art CFD modeling is capable to reproduce this phenomenon as it is visualized for the three investigated fuel blends in Fig. 10.

Approximately 2ms after the start of injection a quasi steady-state concerning lift-off length can be observed in all three cases. A comparison of the lift-off lengths at this instant for the diverse fuel blends ($LOL_{100\%}$=25.25mm,

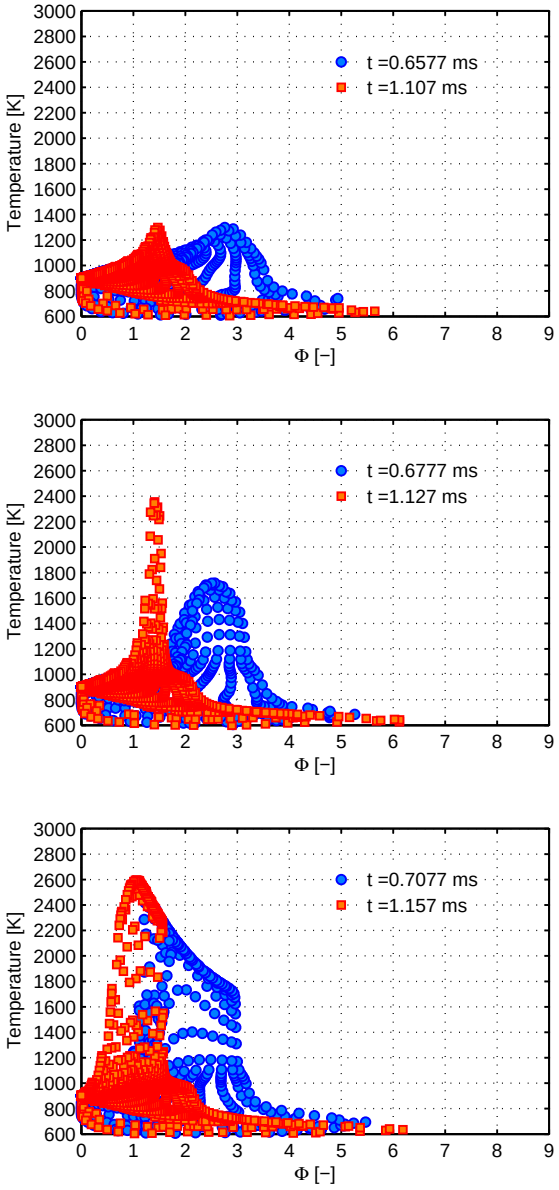

Figure 9: Effect of the fuel proportion on the ignition process. Circles: pure diesel, squares: 60/40 diesel-gasoline blend. Top figure: at start of combustion (SOC), middle figure: 0.02ms after SOC, bottom figure: 0.05ms after SOC

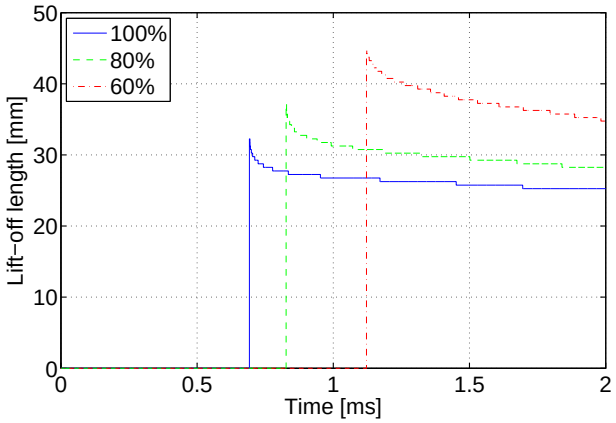

Figure 10: Comparison of the temporal evolution of lift-off length

$LOL_{80\%}$=28.25, $LOL_{60\%}$=34.75mm), shows a non-linear correlation between diesel proportion and LOL. A progressive increase in lift-off length for fuel blends with higher gasoline proportion can be found. So modifying the fuel reactivity provides the possibility to adjust the lift-off length and as a consequence also the flame structure.

The high interest in controlling the lift-off length arises from its relationship with the pollutant formation during combustion [38]. Several strategies exist to control the lift-off length, such as reducing the ambient temperature, decreasing the injector hole diameter or increasing the injection pressure in order to increase the lift-off length. The implementation of these strategies in real engines is difficult and/or expensive. Therefore, controlling the lift-off length by adjusting the fuel reactivity is a promising approach.

The CFD simulation results shown in Fig. 11 illustrate the above mentioned change in flame structure. The color range represents the equivalence ratio. In the exact same manner as in the images shown in the previous subsection, temperature contours for T>1300K are depicted in a plane through the spray axis. Additionally, the white line plotted in the figure indicates a threshold of OH mass fraction. OH mass fraction has been used to determine the lift-off length of the flame as it is done in experimental investigations [36, 39].

Especially when comparing pure diesel fuel versus the 60/40 diesel-gasoline blend as shown in Fig. 11, the difference in flame structure is noticeable. It is important to point out that the reacting zone of this fuel blend does not

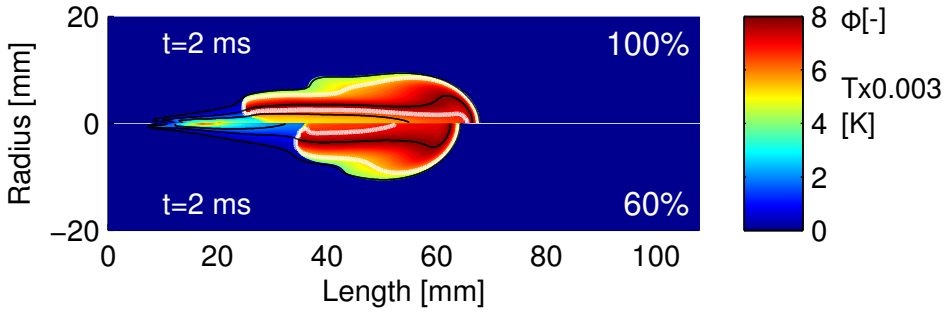

Figure 11: Flame structure comparison. Pure diesel (top half), 60/40 diesel-gasoline blend (bottom half)

reach rich mixture regions. On the contrary, in the pure diesel fuel spray some parts of the rich mixture (inner black line marking ϕ=2) enter the high temperature region. The consequence of this fact is illustrated in the ϕ-T-map in Fig. 12, where temperature is depicted versus equivalence ratio. Additionally, the soot region is marked in the figure. Both the 60/40 and the 80/20 dual fuel blends show potential to avoid generating a sooting flame during combustion.

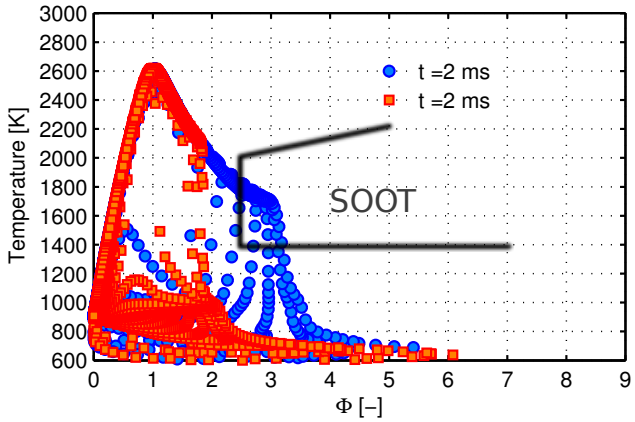

Figure 12: ϕ-T map and soot region. Pure diesel (circles), 60/40 diesel-gasoline blend (squares)

5. Conclusions

A theoretical investigation based on CFD modeling has been performed with the aim of evaluating the impact of fuel reactivity on the characteristics

of a diesel-like reacting spray. Starting from a reference diesel (n-heptane) spray, two additional sprays were modeled decreasing the fuel reactivity by increasing the proportion of gasoline (iso-octane) in the dual fuel blend. According to the results of this research the following outcomes can be summarized:

- Controlling the fuel reactivity by means of blending fuels with different chemical characteristics, such as diesel and gasoline, represents an attractive alternative for adjusting the characteristics of a reacting spray.
- The expected dependence of modified fuel reactivity on the ignition delay was confirmed, but also the impact on the flame structure along the diffusion-controlled combustion process was shown.
- The flame lift-off length, which is directly related to soot formation, was observed to be intrinsically related to fuel reactivity.
- The final impact on the flame structure was evidenced in terms of the equivalence ratio-temperature maps, since the reacting zones of the spray were shifted toward lower equivalence ratios, avoiding the zones of soot formation.

The suitability of combining state of the art CFD modeling tools together with a convenient chemistry model in terms of size and accuracy for reproducing the complex physical and chemical processes involved in dual fuel reacting sprays has been proven. Consequently, CFD modeling provides detailed qualitative spatial information about the local thermo-fluid dynamic conditions inside the spray and their time evolution. The expected trends in key parameters, such as ignition delay and flame lift-off length, as well as the effect on the equivalence ratio-temperature maps were well described by CFD results.

Acknowledgement

The authors want to thank Dr. José Manuel Pastor for his support during this work and for sharing his profound knowledge and experience. Support for this research was provided by the Universidad Politécnica de Valencia inside the program named *Programas de Apoyo a la I+D+I, Primeros proyectos*

de investigación (reference PAID-06-11 2033), which is gratefully acknowledged.

References

[1] G. Banco, An Analysis of the Federal Government's Role in the Research and Development of Clean Diesels in the United States, SAE 2004-01-1753 (2004).

[2] S. Charlton, Developing Diesel Engines to Meet Ultra-low Emission Standards, SAE 2005-01-3628 (2005).

[3] Diesel car sales set to overtake petrol in Europe, Report of PriceWaterhouseCoopers (2006).

[4] H. Yanagihara, Y. Sato, J. Minuta, A simultaneous reduction in NOx and soot in diesel engines under a new combustion system (Uniform Bulky Combustion System - UNIBUS), 17th International Vienna Motor Symposium (1996) 303–314.

[5] S. Kimura, O. Aoki, H. Ogawa, S. Muranaka et al., New Combustion Concept for Ultra-Clean and High-Efficiency Small DI Diesel Engines, SAE Technical Paper 1999-01-3681 (1999).

[6] H. Akagawa, T. Miyamoto, A. Harada, S. Sasaki et al., Approaches to Solve Problems of the Premixed Lean Diesel Combustion, SAE Technical Paper 1999-01-0183 (1999).

[7] G.T. Kalghatgi, P. Risberg, H.-E. Ångström, Advantages of Fuels with High Resistance to Auto-Ignition in Late-Injection, Low temperature, Compression Ignition Combustion, SAE Technical Paper 2006-01-3385 (2006).

[8] G. Kalghatgi, L. Hildingsson, B. Johansson, Low NOx and low smoke operation of a diesel engine using gasoline-like fuels, Proceedings of the ASME Internal Combustion Engine Division 2009 Technical Conference, ICES2009-76034 (2009).

[9] L. Hildingsson, G. Kalghatgi, N. Tait, B. Johansson et al., Fuel Octane effects in the Partially Premixed Combustion Regime in Compression Ignition Engines, SAE Technical Paper 2009-01-2648 (2009).

[10] V. Manente, B. Johansson, P. Tunestål, Partially Premixed Combustion at High Load using Gasoline and Ethanol, a Comparison with Diesel, SAE Technical Paper 2009-01-0944 (2009).

[11] R. Hanson, D. Splitter, R. Reitz, Operating a Heavy-Duty Direct-Injection Compression-Ignition Engine with Gasoline for Low emissions, SAE Technical Paper 2009-01-1442 (2009).

[12] K. Inagaki, T. Fuyoto, K. Nishikawa, K. Nakakita, Dual-Fuel PCI Combustion Controlled by In-Cylinder Stratification of Ignitability, SAE Technical Paper 2006-01-0028 (2006).

[13] P.W. Bessonette, C.H. Schleyer, K.P. Duffy, W.L. Hardy et al., Effects of Fuel Property Changes on Heavy-Duty HCCI Combustion, SAE Technical Paper 2007-01-0191 (2007).

[14] D. Veynante, L. Vervisch, Turbulent Combustion Modeling, Progress in Energy and Combustion Science 28 (2002) 193–266.

[15] R. D. Reitz, C. J. Rutland, Development and Testing of Diesel Engine CFD Models, Progress in Energy and Combustion Science 21 (1995) 173–196.

[16] R. Payri, F. Salvador, J. Gimeno, L. Zapata, Diesel Nozzle Geometry Influence on Spray Liquid-phase Fuel Penetration in Evaporative Conditions, Fuel 87 (2008) 1165–1176.

[17] J. Desantes, R. Payri, F. Salvador, J. de la Morena, Influence of Cavitation Phenomenon on Primary Break-up and Spray Behavior at Stationary Conditions, Fuel 89 (2010) 3033–3041.

[18] X. Margot, S. Hoyas, P. Fajardo, S. Patouna, CFD Study of Needle Motion Influence on the Spray Conditions of Single-Hole Injectors, Atomization and Sprays 21 (2011) 31–40.

[19] S.C. Kong, Y. Sun, R.D. Reitz, Modeling Diesel Spray Flame Lift-off, Sooting Tendency and NOx Emissions Using Detailed Chemistry with Phenomenological Soot Model, ASME Journal of Gas Turbines and Power 129 (2007) 245–251.

[20] Y. Ra, R. Reitz, A Reduced Chemical Kinetic Model for IC Engine Combustion Simulations with Primary Reference Fuels, Combustion and Flame 155 (2008) 713–738.

[21] S.L. Kokjohn, R.M. Hanson, D.A. Splitter, R.D. Reitz, Experiments and Modeling of Dual-Fuel HCCI and PCCI using In-Cylinder Fuel Blending, SAE Technical Paper 2009-01-2647 (2009).

[22] Spray A Operating Condition, Engine Combustion Network (ECN), http://www.sandia.gov/ecn/cvdata/sprayA.php (September 2011).

[23] Silicon Graphics International Corp., OpenFOAM: The Open Source CFD Toolbox, http://www.openfoam.com (September 2011).

[24] J. Dukowicz, A Particle-Fluid Numerical Model for Liquid Sprays, Journal of Computational Physics 35 (1980) 229–253.

[25] F. Kärrholm, Numerical Modelling of Diesel Spray Injection, Turbulence Interaction and Combustion, PhD Thesis, Chalmers University of Technology, 2008.

[26] B. Launder, D. Spalding, Mathematical Models of Turbulence, London Academic Press, 1972.

[27] J. Janicka, N. Peters, Prediction of Turbulent Jet Diffusion Flame Lift-off Using a PDF Transport Equation, Symposium (International) on Combustion 19 (1982) 367 – 374.

[28] J. Beale, R. Reitz, Modeling Spray Atomization with the Kelvin-Helmholtz/Rayleigh-Taylor Hybrid Model, Atomization and Sprays 9 (1999) 623–650.

[29] C. Crowe, J. Schwarzkopf, M. Sommerfield, Y. Tsuji, Multiphase Flows with Droplets and Particles, CRC Press, 1997.

[30] R. Novella, A. García, J.M. Pastor, V. Domenech, The role of detailed chemical kinetics on CFD diesel spray ignition and combustion modelling, Mathematical and Computer Modelling 54 (2011) 1706–1719.

[31] G.M. Faeth, L.-P. Hsiang, P.-K. Wu, Structure and Breakup Properties of Sprays, Int. J. Multiphase Flow 21 (1995) 99–127.

[32] T. Lucchini, G. D'Ericco, D. Ettorre, Numerical investigation of the spray-mesh-turbulence interactions for high-pressure, evaporating sprays at engine conditions, International Journal of Heat and Fluid Flow 32 (2011) 285–297.

[33] S. Jerzembeck, N. Peters, P. Pepiot-Desjardins, H. Pitsch, Laminar burning velocities at high pressure for primary reference fuels and gasoline: Experimental and numerical investigation, Combustion and Flame 156 (2009) 292–301.

[34] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, A Comprehensive Modeling Study of iso-Octane Oxidation, Combustion and Flame 129 (2002) 253–280.

[35] L. M. Pickett, D. Siebers, C.A. Idicheria, Relationship Between Ignition Processes and the Lift-off Length of Diesel Fuel Jets, SAE Paper 2005-01-3843 (2005).

[36] D. Siebers, B. Higgins, Flame Lift-off on Direct-injection Diesel Sprays under Quiescent Conditions, Transactions of the SAE 110 (2001) 400–421.

[37] L. M. Pickett, S. Kook, H. Persson, O. Andersson, Diesel Fuel Jet Lift-off Stabilization in the Presence of Laser-induced Plasma Ignition, Proceedings of the Combustion Institute 32 (2009) 2793–2800.

[38] D. S. L.M. Pickett, Soot Formation in Diesel Fuel Jets Near the Lift-off Length, International Journal of Engine Research 7 (2006) 103–130.

[39] C. Pauls, G. Grünefeld, S. Vogel, N. Peters, Combined Simulations and OH-Chemiluminescence Measurements of the Combustion Process using Different Fuels under Diesel-Engine like Conditions, SAE Paper 2007-01-0020 (2007).