Fuel Composition Influence on Auto-ignition in 3D Engine Simulations

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Introduction

Progress in engine design is motivated by the emergence of environmental regulations. The use of numerical models is now seen as an essential stage both for physics understanding and predictive applications. New injection strategies used in Diesel or gasoline engines together with new combustion strategies such as HCCI (Homogeneous Charge Compression Ignition) have risen interest for 3D auto-ignition modeling. New auto-ignition models relying on detailed chemistry approaches have appeared. They are used directly or in a semi-reduced form in very simple combustion chamber configurations as described in the work of Barths *et al.* (1999) or Kraft *et al.* (2000). Starting from the knowledge of fully detailed chemical mechanisms, various methodologies have been proposed to tabulate complex chemistry, among which FPI (Flame Prolongation of ILDM, Gicquel *et al.* (2000)), ISAT (In-Situ Auto-ignition Tabulation, Pope (1997)), FGM (Flamelet-Generated Manifold, van Oijen *et al.* (2001)). The TKI model (Tabulated Kinetics of Ignition, Colin *et al.* (2005)) used in the following developments has common features with FPI but is originally designed for auto-ignition process in engines.

In this work, we test the sensitivity of the auto-ignition characteristics to a Diesel surrogate fuel. Despite n-heptane is a good candidate in terms of cetane number to represent Diesel auto-ignition more representative fuels should be considered. Firstly, a mixture composed of an alkane and an aromatic is basically tested. Then it is compared to n-heptane in homogeneous configurations with conditions similar to those met in practical engines. Finally, some real engine working points are calculated with pure n-heptane and the mixture using the TKI approach.

Kinetics modeling of a complex Diesel fuel

Practical fuels such as Diesel fuels are multicomponent and consist of such a lot of different chemical species that a detailed modeling of the involved chemical reactions with sufficient accuracy is not possible up to now. First, we consider a fuel mixture composed of n-decane and α-methylnaphthalene which physical and chemical properties are close to those of a real fuel and which was proposed for Diesel auto-ignition in previous studies (Barths *et al.*). The complex mechanism for this mixture is issued from the DCPR (Département de Chimie Physique des Réacteurs, CNRS, France). The n-decane mechanism has been generated with an automatic algorithm for linear alkane oxidation proposed by Warth *et al.* (1998) whereas the α-methylnaphthalene mechanism and its coupling with n-decane is original and has been derived from a reaction manifold written to account for aromatic hydrocarbons (Belmekki *et al.* 2002). The final mixture mechanism contains 3581 reactions and 669 species and is basically validated against experiments in constant volume configurations, such as those presented in Fig. 1. Shock tube results of Pfahl *et al.* (1996) for pure α-methylnaphthalene are compared to complex chemistry calculations at constant volume which are run with the Senkin code. Droplet ignition results of Moriue *et al.* (2000) are used to test
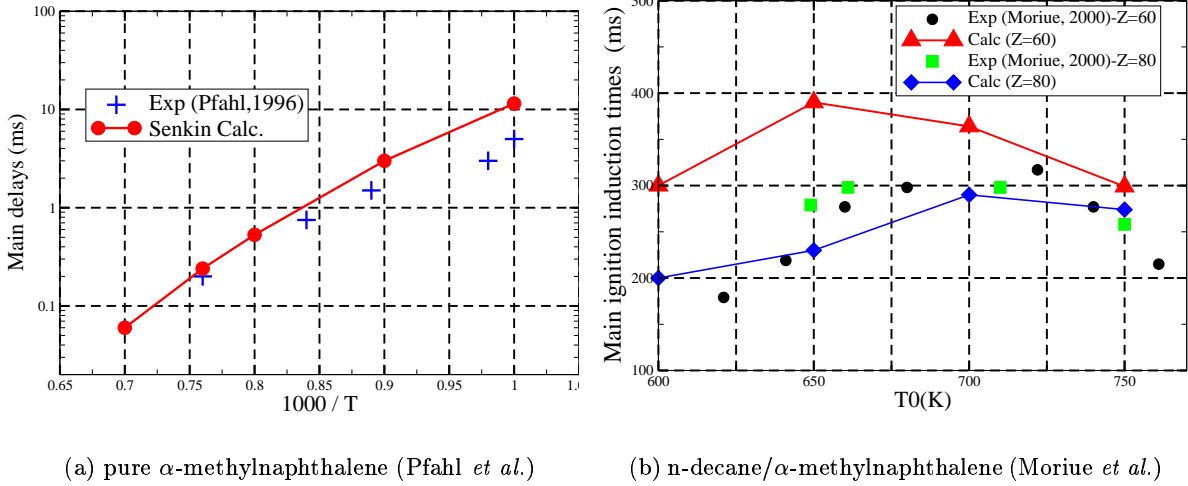
(a) pure α-methylnaphthalene (Pfahl *et al.*) (b) n-decane/α-methylnaphthalene (Moriue *et al.*)

Figure 1: Comparison of delays calculated with the mixture mechanism and different measurements for pure α-methylnaphthalene and n-decane/α-methylnaphthalene.

different n-decane/α-methylnaphthalene mixtures. The main induction delay times are compared for n-decane molar fraction Z=60 % and Z=80 % in Fig. 1 (b). For both cases, the mixture mechanism represents quite well the measured values and the inhibition factor of α-methylnaphthalene is well featured despite the calculated delays overestimate the experimental results.

After these preliminary validations, we compare the relative deviation between the main delays for pure n-heptane and a mixture of 70% volumetric n-decane and 30 % α-methylnaphthalene (Z=70 %). The n-heptane mechanism is issued from the DCPR with the same algorithm as for the n-decane (Warth *et al.*). One can plot the differences between the delays by representing the relative deviations between the two mechanisms along the thermodynamic conditions that one may expect to meet in a real engine. The deviations which are plotted in a (T_0,p_0) diagram for different compositions are differently distributed along all the possible conditions that we tested. We varied the initial temperature T_0 ($T_0 \in [600K, 1500K]$ every 10 K), the initial pressure p_0 ($p_0 \in [1MPa - 8MPa]$), the composition expressed in terms of the global equivalence ratio ϕ ($\phi \in [0.3 - 3]$) and dilution gas fraction X_{res} ($X_{res} \in [0\% - 90\%]$). An exemple of the results obtained is plotted in Fig. 2 (a) for ϕ=1, X_{res}=0 %.

The differences essentially depend on the initial temperature and the pressure influence is small. Nevertheless, the same deviation between two different pressures will result in a more important difference between the delays when the pressure is low (for instance p under 3 MPa) because the delays are longer. The differences between the two fuels are essentially located in a medium temperature range, between 750 K and 900 K (cool flame region) whatever the pressure is. We notice that deviations between the delays can be significant and reach 100 % for these conditions. In these cases, the differences may be important as the delays are large. The deviations rapidly fall above 1000 K to reach values under 10 %. These observations are confirmed by the classical delay plots as a function of pressure and inverse of the temperature (see Fig. 2 (b)). As a result, one may expect that the good prediction of the auto-ignition delays like those obtained by
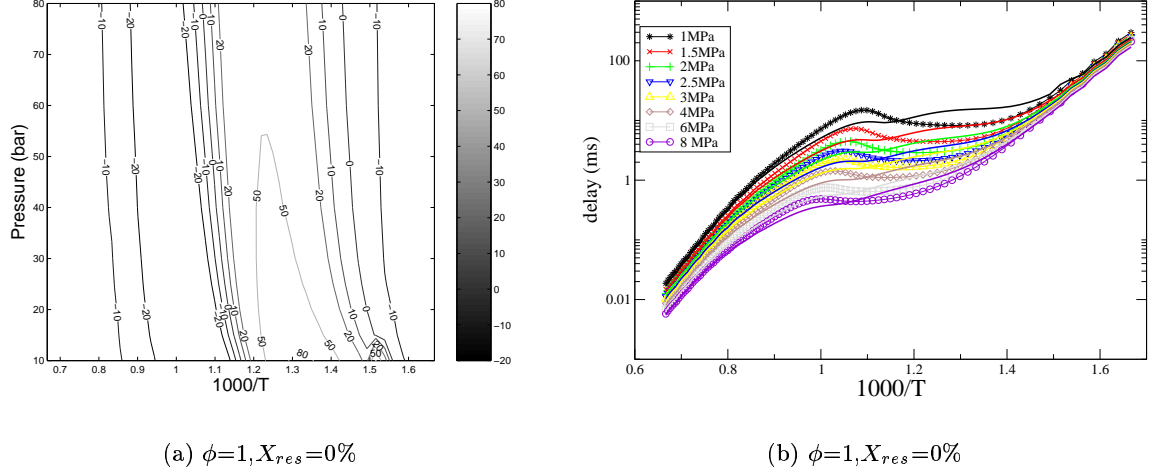
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<center>(a) $\phi=1, X_{res}=0\%$ (b) $\phi=1, X_{res}=0\%$</center>

Figure 2: Comparison of the n-heptane and the mixture n-decane/α-methylnaphthalene (Z=70 %) delays function of 1000/T. Left : Relative deviations between the delays of the two fuels. Right : Pure n-heptane delay curves (symbols) and n-decane/α-methylnaphthalene delay curves (solid lines).

Reveille *et al.* (2004) with pure n-heptane for high temperature auto-ignition will not be affected. When low temperature mechanisms are involved some strong effects can be observed by choosing a n-decane/α-methylnaphthalene mixture.

3D engine simulations

ECFM3z combustion model

For comparisons with experimental engines results, the TKI auto-ignition model presented in Colin *et al.* (2005) allowing to cover a broad range of thermodynamic conditions typical of internal combustion engines is used. The TKI model is integrated in the framework of ECFM3z (Extended Coherent Flame Model-3 zones) presented in Colin *et al.* (2004). We briefly summarize the principle of ECFM3z which integrates the ECFM (Spark Ignition combustion) and the CFM3z (Diesel combustion) approaches into a unique description. To represent the mixing regions, the ECFM3z model includes a description of the local stratification by considering three regions : one region contains only pure fuel (F), the second region contains a mixture of fuel and air (M) and the third region contains only air+EGR (A). During injection, the evaporation of the spray droplets leads to a source of mass in region F. The fuel in region F begins to mix with the air (with EGR) of region A and they form a mixture in region M (Béard *et al.*,2003). The air+EGR/fuel mixture can then auto-ignite in region M. When the auto-ignition delay is reached, combustion in region M starts which leads to the formation of burned gases in this region. From this instant, the region M is divided into unburned and burned gases zones. As the fresh gases are oxidised by auto-ignition, the hot products formed are added to the burned gases mixing region.
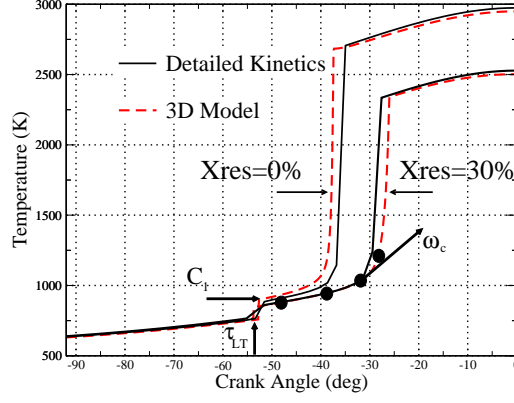
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Figure 3: Comparison of detailed kinetics (Senkin) with TKI model in rapid compression machine (1200 rpm, $\phi = 1$, $X_{res} \in \{0\%; 30\%\}$). The TKI tabulated parameters (τ_{LT},C_1,$\dot{\omega}_c$) are indicated.

TKI auto-ignition model

The TKI model relies on the *a priori* construction of a database of reaction rates for the progress variable c from complex chemistry simulations. It has been validated in homogeneous configurations against complex chemistry and applied to the simulation of conventional Diesel and HCCI combustion. First, the cool flame description included in this approach consists in interpolating a cool flame delay τ_{LT} and a cool flame consumption fraction C_1 in the database. As in Pires da Cruz (2004), the cool flame delay is calculated through integration of an intermediate species Y_I. The growth rate of $\widetilde{Y_I}$ is proportional to the cool flame ignition delay. When it reaches the value of one, the cool flame delay is reached and the cool flame fraction C_1 is consumed rapidly. Then, the main ignition is modeled with tabulated reaction rates $\dot{\omega}_c$ as a function of a progress variable c. The tabulated data are indicated in Fig. 3 comparing the results given by the model with detailed kinetics in homogeneous test cases (rapid compression machine).

Simulation results

The simulations performed with the IFP-C3D code (Zolver *et al.*, 2004) are presented in Fig. 4. Two different engines are considered. The main characteristics are gathered in Tab. 1. The fuel injected has thermodynamic properties corresponding to a practical fuel. Only the kinetics is changed (either the pure n-heptane or the mixture Z=70 %) and the detailed mechanisms are those tested in the previous section. Figure 4 (a) compares the experimental pressure curve of a partial load, diluted (EGR=30%) direct injection Diesel engine with the pressure curves computed with n-heptane and with the mixture fuel. One can see only little difference on the auto-ignition process. Figure 4 (b) corresponds to a HCCI (EGR=50%) split injection engine. The mixture fuel delay is longer than the n-heptane delay which, in this case, seems to be in better agreement with the experiment. One can deduce from these results that the simulations are more sensitive to the kinetics in HCCI conditions where delays are usually longer. The use of detailed reactions representative of gasoil fuel is essential in those conditions because large deviations of delays and reaction rates may be observed between different surrogate fuels. At this stage of our development, the choice of a surrogate fuel that could match practical fuels in all operating conditions needs

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| Parameter	*split injection* HCCI engine	*single injection* conventional engine
BMEP	0.5 MPa	0.37 MPa
RPM	1500	1640
Bore	8.7 cm	8.5 cm
Stroke	9.2 cm	8.8 cm
Connecting rode	14.99 cm	14.5 cm
Compression ratio	14	17.8
Injection start	9 ca et -11 ca BTDC	6 ca BTDC
Injection duration	3.79 ca et 3.54 ca	8 ca
Injection pressure	140 MPa	96 MPa
Injected mass	3.83 mg	2.446 mg
T_0	426 K	460 K
P_0	0.168 MPa	0.1175 MPa
EGR rate	50 %	31 %

Table 1: Main parameters of the 3D computations (BMEP : Break Mean Effective Pressure - RPM : Revolutions Per Minute - EGR : Exhaust Gas Recirculated).

further investigations. Indeed, n-heptane has a cetane number (CN_{nc7}=56) close to those of real Diesel fuels which makes it a good candidate for Diesel auto-ignition modeling. On the contrary the mixture Z=70 % envisaged in this work has a cetane number of $CN_{Z=70}$=53.2 determined from the linear correlation of Kalghatgi (2005). This value is also close to the cetane number of practical Diesel fuels, which is consistent with the results obtained in this section, namely the same high temperature behaviours but different low temperature behaviours. Experiments using different hydrocarbon mixtures running on an engine test bench would help to determine a model fuel for the simulations and an appropriate criterion to characterize auto-ignition at low temperatures.
Figure 5 shows the temperature fields in the 3D computed sector at the onset of combustion (maximum pressure gradient after auto-ignition start). One can notice that the temperature field in the HCCI engine is more homogeneouly distributed in the chamber and takes lower values than in the conventional engine. In this last case auto-ignition occurs in a more restricted region in the top of the bowl. On the contrary the HCCI case features a more extended auto-ignition region. One can see how the flame structure is modified when one switched from a conventional Diesel combustion engine to a HCCI type engine with higher dilution rates and a split injection strategy. Another important point is that the fuel/air ratio distributions in the chamber (see Fig 6) is of first order for the auto-ignition prediction. This may explain why the differences obtained between the fuels in homogeneous configurations may vanish in the case of real practical engines simulations. Nevertheless, the lower temperature fields in HCCI conditions strongly justify the particular attention paid to cool flames description included in the surrogate fuel kinetic modeling and in the engine auto-ignition 3D model.
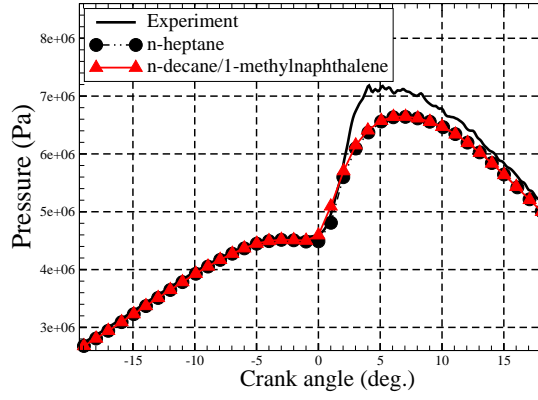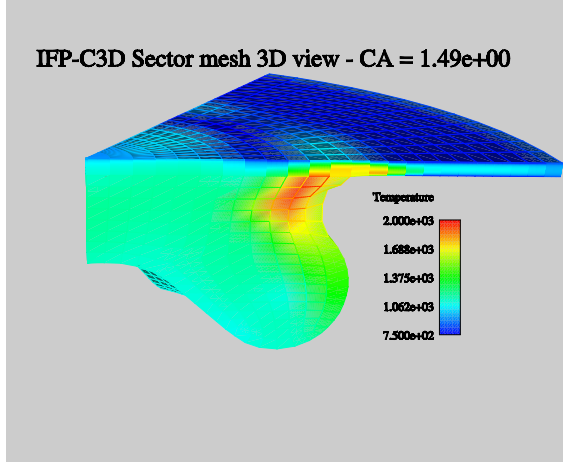
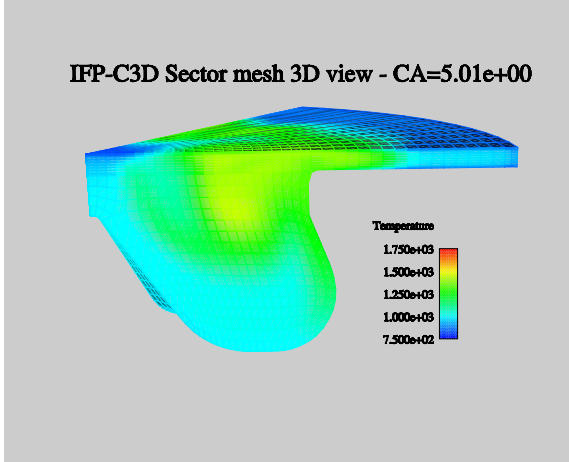(a) 1640 RPM, BMEP 3.7 bar, EGR=31 %
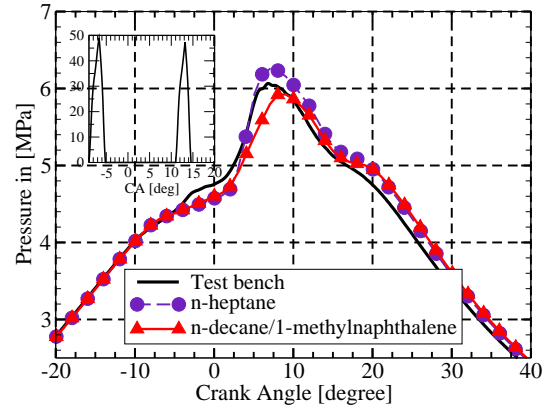
(b) 1500 RPM, BMEP 5 bar, EGR=50 %

Figure 4: Engine 3D simulations. Comparison of the pressure evolution using n-heptane and n-decane/α-methylnaphthalene (Z=70 %).
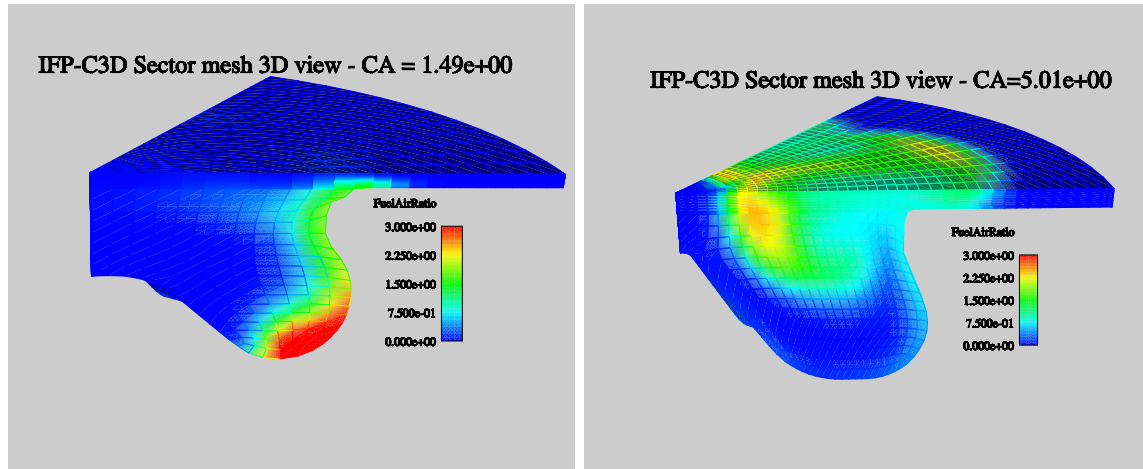

(a) 1640 RPM, BMEP 3.7 bar, EGR=31 %

(b) 1500 RPM, BMEP 5 bar, EGR=50 %

Figure 5: Engine 3D simulations. Comparison of the temperature fields obtained with the mixture n-decane/α-methylnaphthalene (Z=70 %) when auto-ignition occurs.

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(a) 1640 RPM, BMEP 3.7 bar, EGR=31 %   (b) 1500 RPM, BMEP 5 bar, EGR=50 %

Figure 6: Engine 3D simulations. Comparison of the equivalence ratio fields obtained with the mixture n-decane/α-methylnaphthalene (Z=70 %) when auto-ignition occurs.

Conclusions

The modeling of a complex Diesel fuel as a mixture composed of n-decane and α-methylnaphthalene has been considered. A delay sensitivity analysis along initial thermodynamic conditions, using detailed kinetics mechanisms for two fuels (n-heptane and 70 %/30% n-decane α-methylnaphthalene mixture) has been proposed and the deviations have been analysed. It was shown that the auto-ignition process is similar with the mixture fuel and with n-heptane in classical late injection strategies even at part load diluted conditions. On the contrary, for HCCI engines at lower pressure and temperature the auto-ignition process is more sensitive to the fuel auto-ignition characteristics. It seems that an accurate description of the chemical reactions becomes essential in HCCI conditions. Moreover one may expect from a detailed description of the fuel a better prediction of the whole chemical process including auto-ignition and pollutant formation.

Acknowledgments

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