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MULTICOMPONENT DESCRIPTION OF DIESEL FUEL AND INFLUENCE ON COMBUSTION MODELLING IN DID ENGINES

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ABSTRACT

Designing combustion and injection strategies that reduce engine-out pollutant levels requires the use of three dimensional CFD modelling combined with an accurate description of fuel composition. The influence of the Diesel fuel description (single or multicomponent) on the characteristics of high pressure Diesel sprays and on combustion in direct injection Diesel (DID) engines is studied. Using a Diesel fuel lumping model, two different fuels were computed : "dfl1" with only one pseudo-component and "dfl2" with two pseudo-components. With the "dfl2" fuel, the distribution of the vapor of each pseudo-component is simulated using a multicomponent evaporation model implemented within the multidimensional IFP-C3D code. Comparisons were conducted both in a high pressure cell and in DID engines under standard and HCCI (Homogeneous Charge Compression Ignition) operating conditions. Comparisons between "dfl1" and "dfl2" fuels show that the global characteristics of the Diesel spray in a high pressure cell remain similar although the more volatile pseudo-component evaporates faster for the two component description. Nevertheless, for DID engine full load cases, it appears that this more detailed description of the fuel may have an impact on exhaust emissions, in particular for early injection timings.

INTRODUCTION

As car manufacturers are facing increasingly severe regulations on particulate and NOx emissions from Diesel engines, their efficiency must be improved. Reducing emissions can be achieved by designing combustion and injection strategies that reduce pollutant levels at the engine exhaust port. This requires the use of three dimensional CFD modelling combined with an accurate description of (i) commercial fuel composition to simulate properly local equivalence ratios and (ii) the subsequent combustion and pollutant emissions. However, it is very difficult to model properly the thermodynamic properties of a fuel which contains several hundreds of chemical species. Besides, in the case of Diesel fuels, it is particularly challenging as the properties of many heavy species are not available. The widely used approach consists in modelling Diesel fuels by a single component, such as n-heptane, n-dodecane or the standard "df2" of KIVA-2. More recently, simulations were carried out using a representation of the fuel composition by a continuous distribution function instead of the mass fractions of all the individual components [1, 2, 3, 4]. Unfortunately none of these two approaches are relevant to compute accurately the fuel thermodynamic properties during the whole evaporation process. Thus a new strategy was developed at IFP to find a compromise between a description of the complexity of the fuel mixture and the computing time of a spray. The fuel is lumped into a limited number of pseudo-components using a simple grouping procedure. This alternative strategy was first used to represent commercial gasoline and Diesel fuels by one single pseudo-component [5]. Then it was successfully extended to study knock occurrence in a gasoline direct injection (GDI) engine with three pseudo-components [6].
The aim of this paper is to study the influence of the Diesel fuel description (single or multicomponent) on the characteristics of high pressure Diesel sprays and on combustion in direct injection Diesel (DID) engines. Using a Diesel fuel lumping model, in which the normal boiling temperature of the components is one of the main parameters, two different fuels were computed : "dfl1" with only one pseudo-component [5] and "dfl2" with two pseudo-components. With the "dfl2" fuel, the distribution of the vapor of each pseudo-component is simulated using a multicomponent evaporation model [6] which has been developed within the multidimensional IFP-C3D code [7]. Comparisons between results obtained with "dfl1" and "dfl2" were conducted both in a high pressure cell and in DID engines under typical standard and HCCI operating conditions.

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1 LUMPING PROCEDURE

The lumping procedure into an equivalent single-component fluid or two-component mixture is carried out in two steps. The first step [5], which is the same for both the single and two-component reductions, needs as inputs the Diesel fuel density at 288 K and the true boiling point (TBP) distillation curve[1]. This curve is then split into cuts of equal (narrow) intervals of distillation temperatures (figure 1(a)). For the European commercial Diesel chosen as an example for this study, 21 different cuts are defined corresponding to a temperature interval of 13.7 K. This procedure has been carried out using the PROII^{TM} software (Simsci), which also provides the molecular weight M, critical temperature T_c, critical pressure P_c, acentric factor ω and molar fraction x_i of each cut i.

The second step of the lumping procedure consists in grouping those 21 cuts or pseudo-components into either one or two pseudo-components. The one-component lumping procedure has previously been described [5]. Briefly, the Diesel fuel is represented by a pure pseudo-component with parameters Q (= M, T_c, P_c, ω) calculated from the corresponding parameters of the 21 cuts as follows: $Q = \sum_i x_i Q_i$

The equivalent pure component is referred to as "dfl1" : its approximate global formula is $C_{14.9}H_{29.6}$ and its values of M, T_c, P_c and ω are given in table 1. Those values are required to calculate the thermophysical properties of interest for the engine calculations [5, 6]. The calculation procedure is the same as that used for calculating the properties of the two pseudo-components and will be presented below. In particular, the Peng-Robinson equation of state is used to calculate the phase envelope (figure 1(b)). In the case of a pure compound as "dfl1", the phase rule dictates that this envelope reduces to a single curve in the pressure-temperature plane : this is one of the reasons why we have developed a two-component representation of the Diesel fuel.

As the distribution of (poly-)aromatics in a Diesel fuel is unknown, the only available criterion for the two-component lumping procedure is the distillation temperature : the two-component lump is therefore defined by the boiling temperature separating the "light" pseudo-component from the "heavy" one. In the present case, the use of a lumping procedure [8] leads to the definition of two pseudo-components, the "light" one grouping the first nine components (table 2 of [5]) and the "heavy" one grouping the other 12 components. The corresponding distillation temperature separating the compounds in the "light" and "heavy" cuts approximately corresponds to the distillation temperature of n-tridecane ($C_{13}H_{28}$) : therefore those two cuts or pseudo-components are referred to below as "dfl2a" (C_{13}^-) and "dfl2b" (C_{13}^+) (figure 1(a)). The approximate chemical formula of "dfl2a" and "dfl2b" are $C_{11.58}H_{23.01}$ and $C_{17.45}H_{34.66}$ respectively, and their main parameters are listed in table 1.

The phase envelope of this binary mixture (referred to as "dfl2") has been calculated by the Peng-Robinson equation of state. It is displayed in figure 1(b), where it is compared to the envelope of the European Diesel fuel and to the vapor pressure curves of the pure pseudo-Diesel fuels "dfl1" and "df2". The phase envelope of the two-component "dfl2" fuel is slightly shifted towards higher temperatures (i.e. it is slightly less volatile) compared to the 21-component Diesel fuel, but both envelopes have a similar extension. In contrast to the "df2" of KIVA-2, the vapor pressure curve of "dfl1" lies inside both phase envelopes.

Fuel name	Molar fraction	M (kg/mol)	T_c (K)	P_c (MPa)	ω
df2 (KIVA2)	1.0	0.170	725	1.11	
di (KIVA3)	1.0	0.179	736	2.04	
dfl1	1.0	0.208	717	1.96	0.554
dfl2a	0.44	0.162	665	2.25	0.451
dfl2b	0.56	0.244	759	1.73	0.634

Table 1: Main properties of Diesel pseudo-components.

The global formula and the saturation pressure curve of "dfl1" are both close to those of n-tetradecane (figure 2(a)). But the heat capacity of "dfl1" is lower than that of n-dodecane (figure 2(b)) : this shows that the lumping procedure allows to take into account all the constituting components of the Diesel fuel, for instance aromatics which have a lower heat capacity than normal alcanes.

It appears also that the physical properties of "dfl2a" and "dfl2b" differ significantly from those of "dfl1".

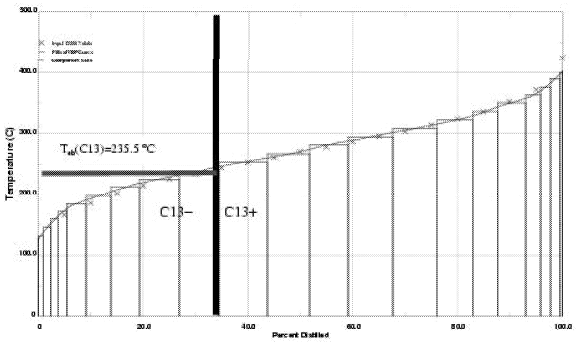
2 3D CFD CODE

Three-dimensional simulations are performed using the multidimensional IFP-C3D code [7]. This code is based on a hexahedral unstructured and parallel formalism. An RNG $k-\varepsilon$ turbulence model is used.

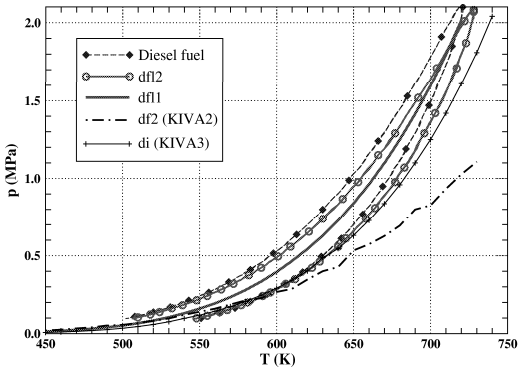
The liquid spray is discretized by the injection of 10 000 computational parcels. Atomization and secondary breakup are computed with the Wave-FIPA model [9]. Collisions and coalescence are neglected as the collision model is strongly mesh dependent. Details of the multicomponent evaporation model can be found in [6] where it was used to study the influence of a multicomponent description of gasoline.

[1] ASTM D2887

Droplet-wall interactions, including evaporation but without the liquid film model, are also taken into account using the model described in [10].
Self-ignition delays are calculated via interpolation inside a database covering a wide range of thermodynamic conditions representative of cold flame ignition as well as main ignition [11]. Combustion is computed thanks to the sub-grid description of the ECFM3Z model developed recently [12]. All the results were obtained without tuning any constant of the combustion model.

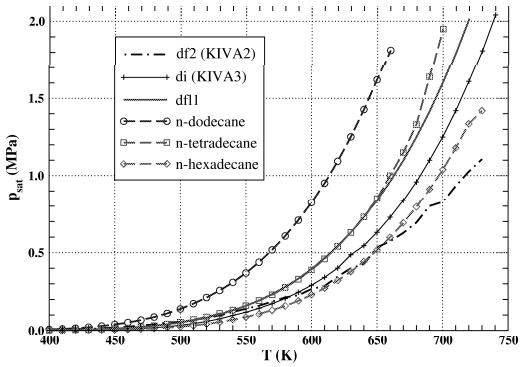


(a) TBP distillation curve (ASTM D2887).

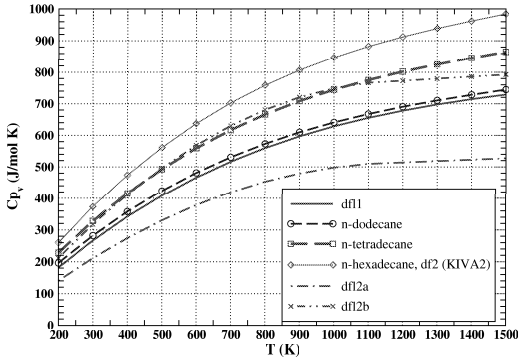


(b) Phase envelopes of the Diesel fuel and "dfl2" and saturation pressure curves of "dfl1" and "df2".

Figure 1: Characteristics of the Diesel fuel.



(a) Saturation pressure.



(b) Isobaric fuel vapor heat capacity.

Figure 2: Comparison of physical properties of various fuels.

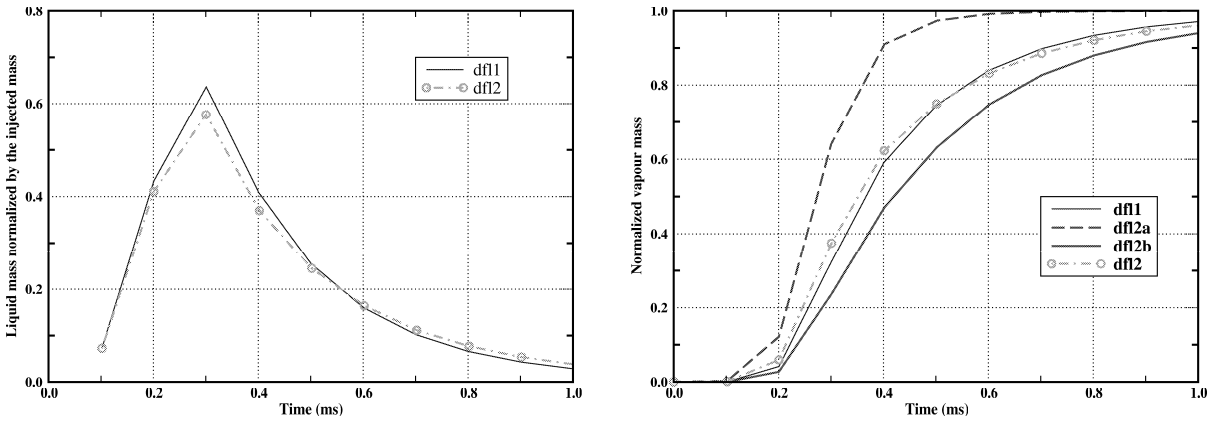
3 HIGH PRESSURE CELL

Simulations were first carried out in a high pressure, high temperature cell which enables to study the spray behaviour under thermodynamic conditions similar to those of a Diesel engine. As in [5], the operating conditions were chosen to be similar to those of a pilot injection (table 2) because at these ambient conditions the evaporation rate is moderate and the differences between the different Diesel fuels should be enhanced.

p_{inj} (MPa)	Δt_{inj} (ms)	m_{inj} (mg)	p_{ch} (MPa)	T_{ch} (K)
80	0.35	4	0.5	600

Table 2: Operating conditions in the high pressure cell.

At the beginning of the injection the liquid mass is the same for "dfl1" and "dfl2" (figure 3(a)). After $0.2\,ms$, the "dfl2" evaporates faster due to the fast evaporation of its light component "dfl2a" (figure 3(b)). Although the molar fraction of this more volatile component in the Diesel fuel is lower than the molar fraction of "dfl2b" (table 1), its vapor mass is higher until the spray impinges the wall of the cell at $t = 0.4\,ms$: this might lead to a shorter ignition delay for combustion conditions. It is observed that neither the liquid penetration nor the vapor penetration is modified by the description of the Diesel fuel. At $t = 1\,ms$, both pseudo-components are vaporized and their respective fractions are close to their initial values in the injected liquid fuel (table 1).



(a) Liquid (b) Vapor

Figure 3: Effect of Diesel fuel description on the temporal evolution of liquid and vapour mass of the different components normalized by their injected mass.

4 DID ENGINE

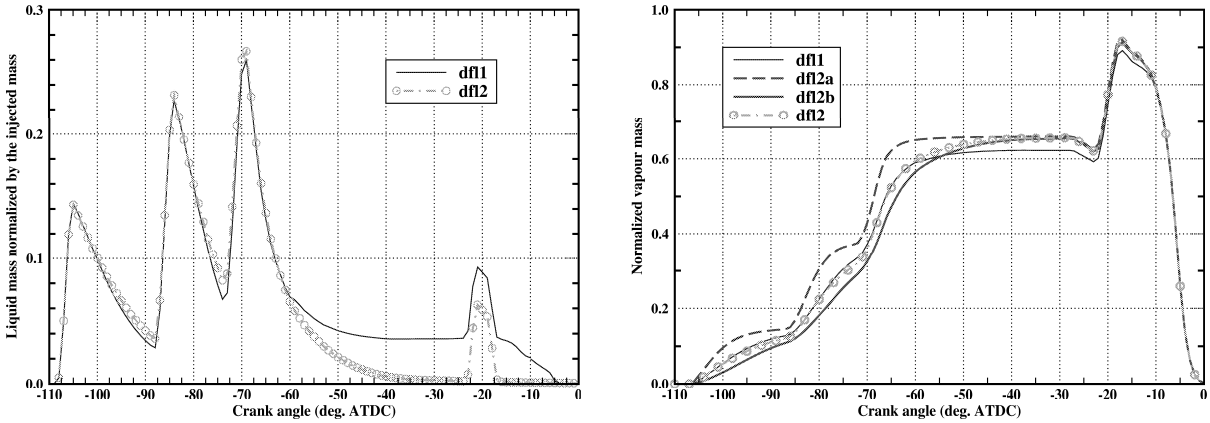
Calculations were performed on 4-stroke DI Diesel (DID) engines for two typical full load operating conditions (table 3). As the six hole injector is located on the axis of the cylinder, only a 60 ° sector of the combustion chamber was considered.

Case	A				B
Engine speed (rpm)	2500				4000
Global equivalence ratio	0.9				0.71
Start(s) of injection (deg. BTDC)	110	90	75	25	15
Exhaust Gas Recirculation (%)	54				0

Table 3: Operating conditions in the DID engines.

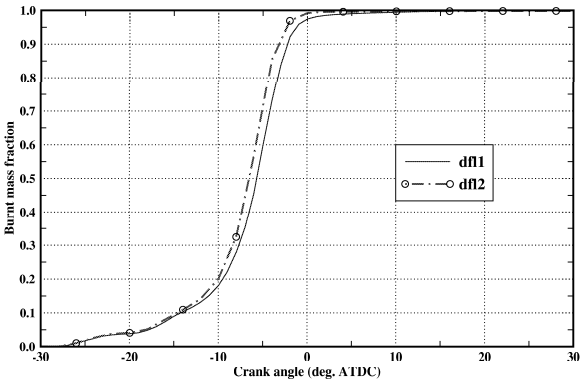
4.1 HCCI Case

The first case (case A) is an HCCI case with four injections. Figure 4 shows that the light component "dfl2a" still evaporates faster leading to a higher liquid mass of "dfl1" than "dfl2" at the end of the compression stroke. As a consequence, the fuel/air mixing is more homogeneous and the combustion is faster with the "dfl2" than with the "dfl1" (figure 5(a)). The description of the Diesel fuel modifies the temperature field in the cylinder and thus exhaust emissions : with the "dfl2", soot mass at exhaust valve opening (EVO) is 2.7 times lower and NO mass increases by 46 % (figure 5(b)), resulting in a noticeable change in soot-NOx emissions trade-off.

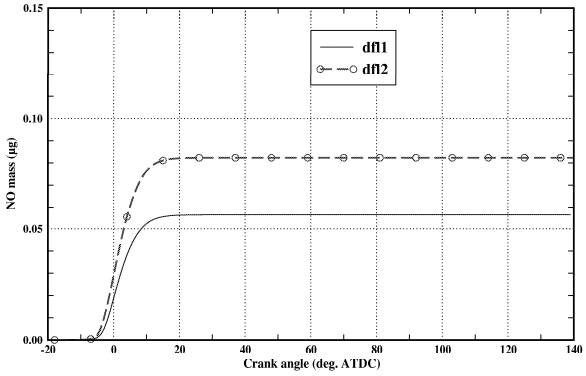


(a) Liquid (b) Vapor

Figure 4: Effect of Diesel fuel description on the temporal evolution of liquid and vapour mass of the different components normalized by their injected mass (case A).



(a) Burnt mass fraction

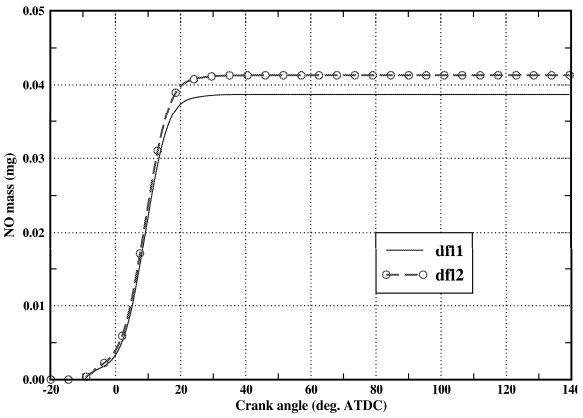


(b) NO emissions

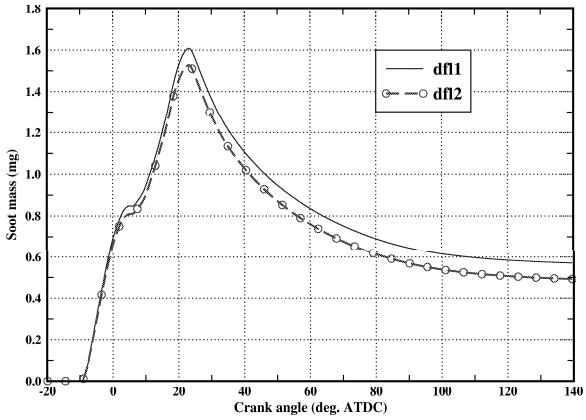
Figure 5: Effect of Diesel fuel description on combustion (case A).

4.2 Conventional Full Load Case

Case B is the full load case previously considered in [5]. In this case, high ambient temperature and pressure lead to fast evaporation of fuel droplets, so liquid and vapor mass as well as combustion remain unchanged using either Diesel fuel representation. Nevertheless it appears that in this configuration the description of the fuel composition may have an impact on pollutant emissions. With the "dfl2", NO mass in the cylinder at EVO increases by 7 % whereas soot mass decreases by 15 % compared to those predicted with the "dfl1" (figure 6).



(a) NO



(b) Soot

Figure 6: Effect of Diesel fuel description on pollutant emissions (case B).

CONCLUSION

An accurate description of fuel thermodynamic properties is required to improve the prediction of fuel/air mixing, combustion and pollutant emissions using a 3D CFD code. In this paper, a Diesel fuel lumping model, in which the normal boiling temperature of the components is one of the main parameters, is presented. Using this lumping procedure to a European commercial Diesel fuel, two different fuels were computed : "dfl1" with only one pseudo-component and "dfl2" with two pseudo-components. With the "dfl2" fuel, the distribution of the vapor of each pseudo-component is simulated using a multicomponent evaporation model which has been developed within the multidimensional IFP-C3D code [7]. Then the influence of the Diesel fuel description (single or bi-components) on the characteristics of high pressure Diesel sprays and on combustion was studied. Comparisons were conducted both in a high pressure cell and in direct injection Diesel (DID) engines under standard and HCCI operating conditions. The simulation time is only slightly affected by the number of pseudo-components. Comparisons between "dfl1" and "dfl2" show that the global characteristics of the Diesel spray in the high pressure cell remain similar despite the more volatile pseudo-component evaporates faster for the two-component description. Nevertheless, for DID engine full load cases, it appears that a detailed description of the fuel may have an impact on fuel/air mixing and exhaust emissions.

Further investigations should be carried out to quantify the influence of the Diesel fuel description on a wider range of operating conditions. Besides, other lumping criteria could be used to define other two or three

pseudo-component lumpings in order to better describe specific features of the Diesel fuel (very light and/or heavy fractions for instance) and to emphasize their effects on DID engine simulations.

NOMENCLATURE

C_p	isobaric heat capacity (J/mol K)
m	mass (kg)
M	molecular weight (kg/mol)
p	pressure (MPa)
T	temperature (K)
x	mole fraction
ω	acentric factor
Δt	duration (s)

Subscripts

c	critical
ch	ambient
inj	injection
l	liquid
sat	saturation
v	fuel vapor

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