MODELING AUTOIGNITION IN MODERN D.I. DIESEL ENGINE

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Abstract

In order to investigate the complex phenomena that occur in the evolution of a fuel spray (break up, evaporation, liquid gas interaction, autoignition, wall impingement) a numerical analysis has been carried out. The numerical tool used is a modified version of the well known KIVA3 code, in which new models were introduced to take into account the processes occurring in modern DI Diesel engines due to the higher ambient and injection pressures reached in latest applications.

The predictive capability of the modified code has been evaluated by comparison between experimental and numerical data. The experimental data were provided by Kobory et al. [1], that measured Diesel fuel ignition delay times in a rapid compression machine, using cylinder ambient gas temperature and pressure measurements as diagnostic, investigating the ignition delay dependency on cylinder temperature and pressure.

Comparisons between experimental and numerical results show good predictive capability of the integrated code, confirming that ignition delay decreases if increasing cylinder temperature.

Introduction

Temporal control of combustion in internal combustion engines is one of the most important parameters that affect efficiency, exhaust emissions and noise. In spark ignition (SI) engines electronic ignition timing can be used to control the start of combustion. In Diesel engines fuel ignition is achieved by compression of the charge, and timing of this event is controlled by a variety of factors that include initial gas temperature and pressure at the time of fuel injection, fuel/air mixing rates and fuel cetane number [1]. The liquid fuel injected into the combustion chamber atomizes, evaporates, decomposes, impinges the wall and mixes with air entrained into the spray. The modeling of the combustion process is greatly dependent on the history of fuel droplets: mixture formation in direct injection Diesel engines can be correctly characterized by means of multidimensional approaches if the spray behavior is accurately described. That implies that all the sub-models concerning the mixture formation must account for the effects of high injection pressure and in-cylinder pressure, typical of Direct Injection (DI) Diesel engines.

Numerical tool

The simulations were performed using an improved version of the KIVA3 code [2]. The KIVA3 code solves the three-dimensional equations of chemically reactive flows with sprays. A lagrangian treatment of stochastic particle injection is used for the liquid drops that represent the fuel jet. The fuel enters the computational domain as a coherent liquid column that is artificially divided, by the KIVA3 spray model, into discrete lagrangian material volumes. Each computational parcel represents a group of physically similar droplets that exchange mass momentum and energy with that surrounding air through source terms in the gas phase equations. The liquid jet is so simulated injecting *blobs* with characteristic size equal to the nozzle diameter.

A new droplet-gas momentum exchange model [3] was used in order to reduce spray morphology grid dependence.

To better predict the evolution of the fuel spray in the combustion chamber of modern DI Diesel engines, significant improvements have been brought to the original spray model, taking into account the differences due to the higher ambient and injection pressures reached in latest applications.

Experimental studies have shown [4-7] that flow conditions inside the injection holes strongly affect the liquid core atomization. A phenomenological flow model [8] has been used to simulate the effects of nozzle geometry on fuel injection and spray processes. Because of the high injection pressure, cavitation may occur in injector holes. The collapse of the bubbles formed increases the level of turbulence in the injector, enhancing atomization of liquid jet. The model predicts the occurrence of cavitation and provides the initial conditions for

the spray model: the effective injection velocity and area, associated to the initial blob size. Turbulent kinetic energy and its dissipation rate are also evaluated [9], since they are required input for the atomization model.

A hybrid model for the atomization of the liquid fuel jet was developed and tested in previous work [10]. It distinguishes between jet primary breakup and droplet secondary breakup. The WAVE [11] model is based on a stability analysis of liquid jets and can be used to simulate the primary atomization of liquid core in the regimes in which jet breakup is governed by aerodynamic interaction with air (low-medium injection pressure case).

In the high pressure case the effects of jet turbulence and cavitation on liquid core primary breakup are considered. The flow model [8] is used to evaluate the occurrence of cavitation and the level of turbulence in the injector. Initial *blob* size, velocity and related κ and ε are estimated. Then Gosman's approach [12] is followed, but, if cavitation does occur, it is taken into account since it affects turbulence and related values of κ and ε in the injector. The model also takes into account exponential growth by Kelvin-Helmholtz (K-H) instabilities due to interaction with air, so the three main mechanisms are considered.

The Taylor Analogy Breakup (TAB) [13] and Droplet and Distortion Breakup (DDB) [14] models are based on the dynamic of single droplet and can be therefore considered as secondary breakup model. In the first the breakup is due to the amplification of droplet deformation resulting from vibrational resonance of the surface and therefore was chosen to model droplet breakup in the Vibrational regime. The latter is a deformation-induced secondary breakup model and used in the Bag regime. The WAVE model is based on the physics of a liquid column (primary breakup) but, since it considers K-H instability effects it can be also used to simulate the breakup of secondary droplets in those regimes in which it may be ascribed to the shear forces at the interface. It was chosen to model the secondary breakup in the Stripping regime and in the Catastrophic one in competition with the Rayleigh-Taylor (R-T) model (Table 1). The R-T model [15] considers Rayleigh-Taylor instabilities that arise on very high speed droplet surface and therefore can be adopted to model droplet secondary breakup in the catastrophic regime in competition with a K-H instability based model (WAVE). In the Chaotic regime, in which bag breakup and stripping coexist, a competition between the DDB model and the Wave model was implemented.

All the models were used with the original value of the constants except for the WAVE model. For the latter customized value of the size constant (B_0=0.59), was chosen according to a previous work [3], while the time constant was set equal to 80 for the low injection pressure range and 15 for the high injection pressure range [10].

HYBRID ATOMIZATION MODEL	
PRIMARY BREAKUP	
Low-Medium injection pressure	WAVE
High injection pressure	Turbulence-cavitation-aerodynamic-induced model
SECONDARY BREAKUP	
12<We<16 (vibrational)	TAB
16<We<45 (bag)	DDB
45<We<100 (chaotic)	DDB + WAVE
100<We<1000 (stripping)	WAVE
We > 1000 (catastrophic)	WAVE + RT

Table 1. Hybrid atomization model.

Due to the high pressures reached in the combustion chamber, Spalding's evaporation model, integrated in the original version of the KIVA code can no longer be used. A different evaporation model, following Hiroyasu's approach [16,17] that considers high pressure effects, was adopted to model the evaporation of liquid droplets. Due to the high temperatures reached in the combustion chamber during the injection period, fuel density cannot be considered constant. As far as the vapor-gas mixture is concerned, the simple ideal state equation leads to ineffective description of its behavior, particularly at the high pressure levels reached during compression and combustion processes. As a consequence the Redlich-Kwong equation was used. When considering real conditions, fugacity coefficients must be introduced in order to evaluate the molar fraction of each component present in the mixture. The deviation from ideal behavior exhibits its influence on vaporization enthalpy.

Spray-wall interaction was also modified following Bai and Gosman's approach [18] to take into account the new regimes typical of high Weber number droplets. Assuming wall temperature below boiling point, as is typical in DI Diesel engines and neglecting the effects of neighboring impinging droplets and gas boundary layer on the impingement dynamics, the following impingement regimes occur, as droplet Weber number increases:

Dry wall: *Stick – Spread – Splash*
Wet wall*: Rebound – Spread – Splash*

- In the *Stick* regime, that occurs at very low impact energy, the droplet adheres to the wall in a nearly spherical form.
- In the *Spread* regime, the droplet, that impinges the wall with a moderate velocity spreads out to form wall film.
- In the *Rebound* regime the droplet bounces off the wall after impact.
- In the *Splash* regime, typical of very high impact energy, the droplet breaks up in many fragments. This regime can occur in modern DI Diesel engines, because of the very high injection pressures reached.

The existence of these impingement regimes is governed by parameters characterizing the impingement conditions such as: incident droplet velocity, size, temperature, angle; fluid viscosity and surface tension; wall temperature, surface roughness, and, if present, wall film thickness. In order to deduce which regime will occur, transition criteria, function of the parameters listed above, are provided [18].

The Shell model [19], developed to predict knock in gasoline engines, was used to model autoignition. It uses a simplified reaction mechanism: eight generic reactions based on the degenerate branching characteristics are formulated from five chemical species, three of which are fictitious. Basically the rate constant of each reaction was in the Arrhenius form. The mathematical model for this generalized reaction set contains 26 kinetic parameters. The premise of the Shell model is that degenerate branching plays an important role in determining the cool flame and two-stage ignition phenomena that are observed during the autoignition of hydrocarbon fuel. The kinetic parameters use the values of 90RON fuel [20]. Since they were determined under certain specific conditions, for fixed fuel characteristics, some constants should be considered adjustable when the Shell model is implemented for Diesel ignition modeling. After a sensitivity analysis [21] the following constants were changed: Ef1= -1.6 e+4, Ef2 = -6.7 e+3, Ef3 = 1.23 e+4.

Analysis of results

Experimental measurements were made by Kobori and Kamimoto [1]. Experimental autoignition time was measured realizing a rapid compression machine reported in figure 1, whose geometric characteristics are shown in table 2.

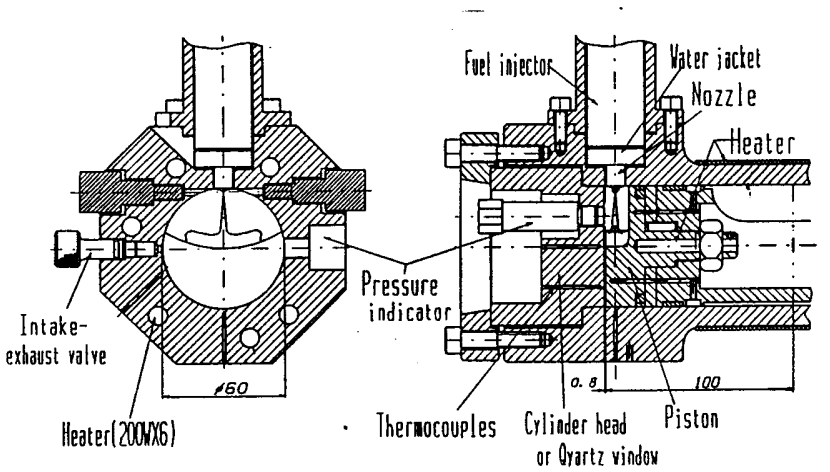

Figure 1. Rapid compression machine scheme

Bore	60 mm
Stroke	100 mm
Displacement	283 cm3
Volume at t.d.c.	17.4 cm3
Compression ratio	17.3
Squish	0.8 mm

Table 2. Geometric characteristics of the rapid compression machine

Case	Pressure	Temperature
#1	42 bar	995 K
#2	42 bar	883 K
#3	42 bar	805 K
#4	42 bar	786 K

Table 3. Tests initial conditions

Fuel is injected in the combustion chamber, at 1000 bar injection pressure and for a duration of 2 ms, through a single hole injector of 0.2 mm diameter. It is evident that the injector operating conditions and the geometry of the chamber are such as to minimize the physical delay allowing the evaluation of the only chemical delay. Ignition delay measurements have been made at different thermodynamic conditions in the combustion chamber as reported in table 3.

Simulations have been made using a 10000 nodes grid, with 1.5 mm grid spacing (figure 2).

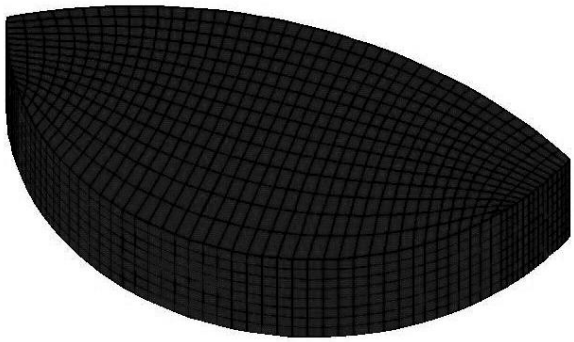

Figure 2. Numerical grid

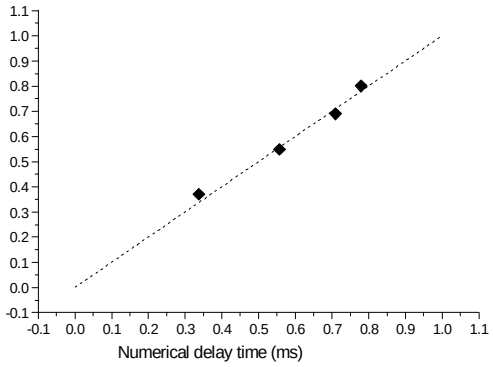

Figure 3. Experimental-numerical ignition delay time

From figure 3, in which the experimental ignition delay time, evaluated as the time (from start of injection) required by the pressure to reach its initial value, are reported as a function of the numerical ones. The good predictive capability of the code can be evinced, being the percentage discrepancy less than 5%.

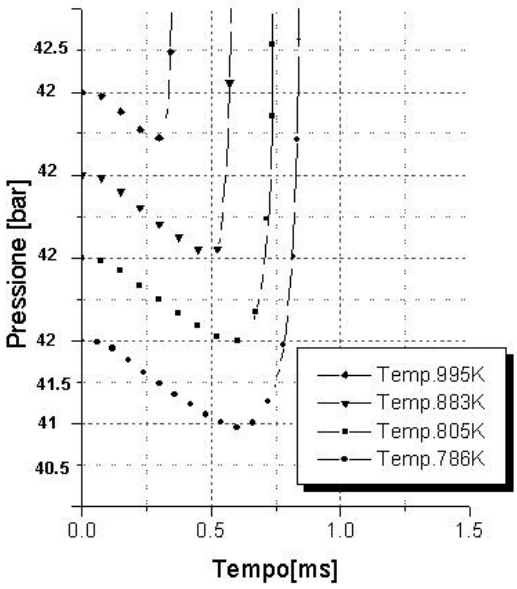

Figure 4. Numerical pressure as a function of time

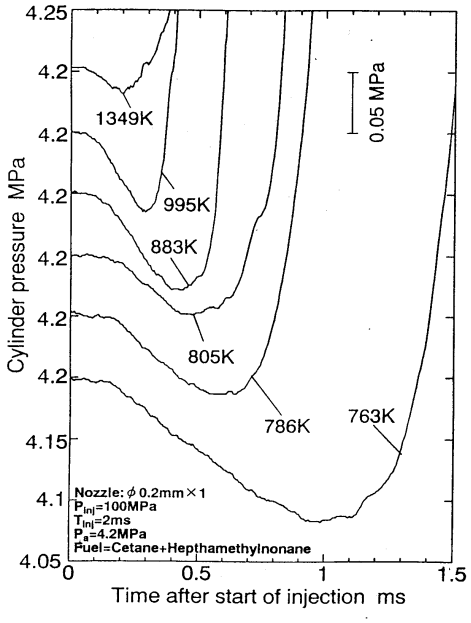

Figure 5. Experimental pressure as a function of time

In figure 4 the numerical values of the pressure, as a function of time, in the four cases are reported. Pressure first decreases because of the heat subtracted by fuel evaporation; then, due to the heat release related to mixture autoignition, suddenly increases reaching an asintotic value. In figure 5 the experimental corresponding values are reported. The comparison of the two figures confirms the good predictive capability of the code for a big range of gas initial temperature (786K÷995K).

After a first evaluation, based essentially on global data, local results are reported in the following. Referring to case 2, in figures 6-8 temperature, air/fuel ratio and velocity maps, in a plane passing through the

spray axis at t=0.5 ms after fuel injection, are reported. In the figures, fuel droplets (not in scale) are also reported. Temperature map (figure 6) shows lower gas temperature in the center of the chamber, where fuel evaporation is higher. Air/fuel ratio distribution (figure 7) shows a very rich central zone delimitated by a stoichiometric one (black line). The velocity map (figure 8) shows the effects of momentum exchange between gas and droplets. The air is accelerated in the spray region reaching velocities near 200 cm/s, while remains still in the peripheral zones. The negative values are due to the frame of reference chosen, which has the positive direction opposite to the injected spray. In figures 9-11 the same maps are reported at t =0.6 ms. Autoignition of the mixture has already occurred, in fact two zones around 1500 K can be noticed. The analysis of figure 10, in which air/fuel ratio is reported, shows the presence of high temperature also in zones with very high air/fuel ratio. This can be explained analyzing the velocity field (figure 11) that clearly shows that in the last part of the chamber two vortices arises, making the hot gases flow in the direction of the cold ones. The droplets that impinge on the wall are captured by the vortices, increasing the mixture formation rate. The increase of temperature in these zones is related mainly to convective phenomena.

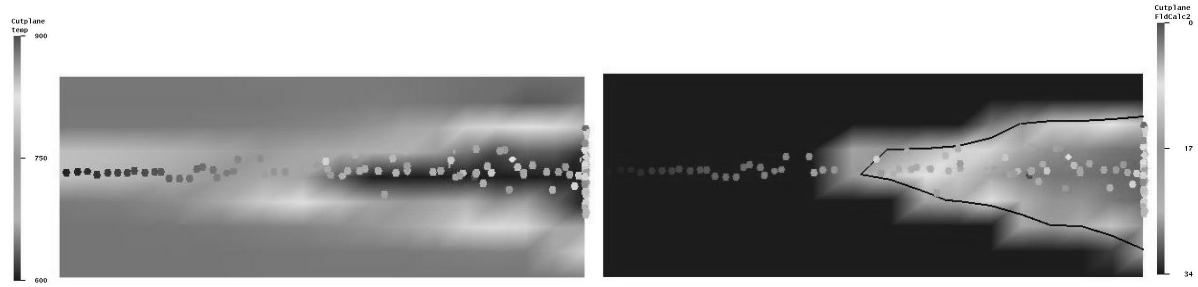

Figure 6. Temperature in a vertical plane passing through the spray axis at t=0.5 ms. Case 2

Figure 7. Air/fuel ratio in a vertical plane passing through the spray axis at t=0.5 ms. Case 2

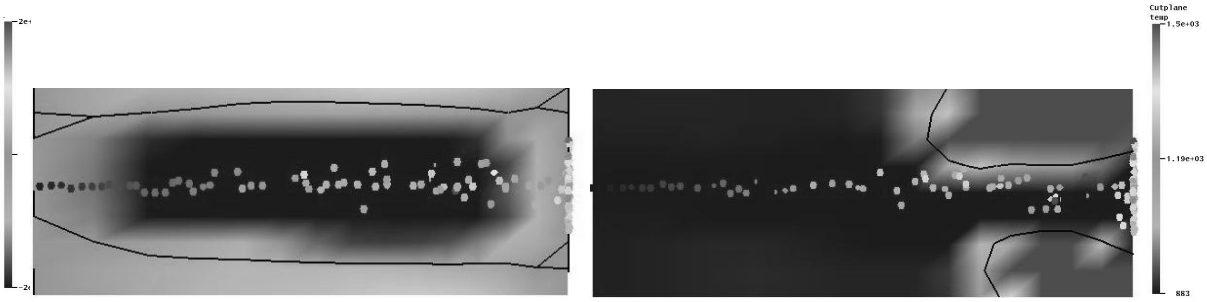

Figure 8. Velocity in a vertical plane passing through the spray axis at t=0.5 ms. Case 2

Figure 9. Temperature in a vertical plane passing through the spray axis at t=0.6 ms. Case 2

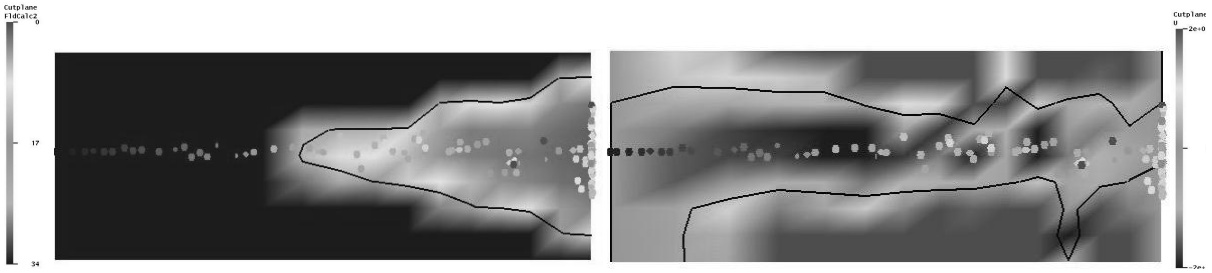

Figure 10. Air/fuel ratio in a vertical plane passing through the spray axis at t=0.6 ms. Case 2

Figure 11. Velocity in a vertical plane passing through the spray axis at t=0.6 ms. Case 2

Conclusions

An integrated model for Diesel ignition has been proposed in this study. Good levels of agreement were obtained between computed and measured data concerning ignition delay time in a rapid compression machine.

The proposed integrated model takes into account the effects of high injection pressure and high in-cylinder pressure in spray evolution, upgrading the spray injection, spray atomization, evaporation and wall-impingement models. For the modeling of the autoignition process the Shell model was used with customized values of the constants.
Further work on mixture formation prediction in high injection Diesel engines will now be made.

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