Numerical and Experimental Analysis of Main Intermediate Species in the Diesel Autoignition Process

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The role of intermediate species participating the low temperature hydrocarbon oxidation in Diesel combustion is investigated by means of a synergetic employment of the KIVA-3 code and optical measurements of flame intensity performed on an optically accessible engine.

From the experimental point of view, various operating conditions corresponding to different crank angles of pressure start of combustion (PSOC) are considered in order to investigate if recording the instant of first appearance of recognisable radicals in the flame intensity spectra and computing the minimum of the indicated pressure trend are equivalent to the scope of determining ignition delay. In all the considered cases it is found that the first stage of combustion is characterised by a weak emission, mainly in the ultraviolet-visible range, attributed to natural chemiluminescence and exhibiting peaks at wavelengths which are typical of OH and CH radicals. Since the flame intensity is proportional to the concentration of the emitting species, the reconstruction of the radicals distribution within the combustion chamber is suitable to be recovered, thus furnishing reliable information about the location of the early combustion spots in both a temporal and a spatial sense.

From a numerical point of view, being the contribution of the chemical delay to the overall amount sufficiently small, multidimensional modelling containing a reduced kinetic scheme is allowed. Ignition delay, in fact, comprises of both a physical and a chemical part, the former due to time needed for spray atomisation, evaporation and mixing with the surrounding air, the last being a function of the burning mixture composition, temperature and pressure. Based on experimental results, an identification of the species involved into the kinetic model, previously considered as fictitious, is supplied. Correspondence is proven, in particular, between the iso-level curves of OH emission intensity and the branching agent concentration entering the model, especially in correspondence of the PSOC for all the simulated operating conditions.

The way fuel evaporation and mixing with air affect the cool flame regime is highlighted by observing typical simulated shapes of the jet and the surrounding vapor region, as the one represented in figure 1, which corresponds to the situation in the chamber as occurring at a crank angle of 4° after the start of injection. The combustion chamber, connected to the main cylinder by a tangential duct of 1
cm in diameter, has a diameter of 3 cm, and the fuel injector is located in a central top position within the chamber. Compression of air into the main cylinder makes for a strong counter-clockwise flow to arise, strongly deviating the fuel spray and the vapor distribution, as highlighted by the represented iso-level surface of vapor concentration. An idea of the size of the employed grid, having a total of 44367 computational cells, is also given. A two-dimensional view of the fuel jet evolution with time is given in figure 2, where three successive configurations are shown.

Subtraction of heat related to evaporation prevents increase of temperature and favours the cool flame regime as evidenced by figure 3, where the temperature within the combustion chamber is shown for the case of a pressure start of combustion occurring 1° before the top dead centre (BTDC). The temperature field exhibits a minimum in correspondence of the jet tip. Figure 4 shows, in the same conditions the branching agent concentration, with its highest values positioned in the region where the internal rotating flow encounters the entering flow.

**Fig.1.** Split of the mesh, fuel droplets distribution and iso-level surface of fuel vapor concentration 4° after start of injection.

**Fig.2.** Jet evolution at 1°, 2° and 4° after start of injection.
Figure 5 finally shows the reconstructed distribution of the experimentally measured flame intensity at wavelength typical of OH and CH radicals for a pressure start of combustion occurring 1° BTDC. Agreement between OH emissivity intensity and the branching agent concentration is quite good. OH radicals, in fact, should arise as a consequence of branching reactions within the low temperature regime. Moreover, the location of ignition can be characterised, within a local approach, by the occurrence of a maximum in the rate of formation with respect to the time of the branching agent involved in the reduced scheme. In this sense, besides the recovering of the PSOC from a global perspective, the assessed numerical code results a reliable tool in the control of the autoignition process.

**Fig. 3.** Temperature distribution 1° BTDC.  
**Fig. 4.** Branching agent concentration 1° BTDC  
**Fig. 5.** OH and CH experimentally measured flame intensity 1° BTDC.