

A 0D Phenomenological Approach to Model Diesel HCCI Combustion with Multi-Injection Strategies Using Probability Density Functions and Detailed Tabulated Chemistry

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ABSTRACT

More and more stringent restrictions concerning the pollutant emissions of ICE (*Internal Combustion Engines*) constitute a major challenge for the automotive industry. New combustion strategies such as LTC (*Low Temperature Combustion*), PCCI (*Premixed Controlled Compression Ignition*) or HCCI (*Homogeneous Charge Compression Ignition*) are promising solutions to achieve the imposed emission standards. They permit low NO_x and soot emissions via a lean and highly diluted combustion regime, thus assuring low combustion temperatures.

In next generation of ICE, new technologies allow the implementation of complex injection strategies in order to optimize the combustion process. This requires the creation of numerical tools adapted to these new challenges.

This paper presents a 0D Diesel HCCI combustion model based on a physical 3D CFD (*Computational Fluid Dynamics*) approach. The purpose of the model is to correctly predict the characteristics of auto-ignition and heat release for all Diesel combustion modes. A new formalism based on PDFs (*Probability Density Functions*) is proposed to describe the mixture formation process in a multi-injection strategy context. This formalism has been coupled with detailed tabulated chemistry to account for the impact of the EGR (*Exhaust Gas Recirculation*) on the kinetics of combustion. The model is finally validated against experimental data.

Considering the good agreement with the experiments and the low CPU costs, the presented approach is revealed to be promising for global-system simulations.

INTRODUCTION

Because of increasing strict limitations on pollutant emissions, car manufacturers are constantly investing more money into the R&D (*Research and Development*) sector in order to improve engine performance. Concerning CI (*Compression Ignition*) engines, the most retained idea, in order to contain pollutant emissions, is to shift from conventional Diesel combustion towards new types of combustion regimes.

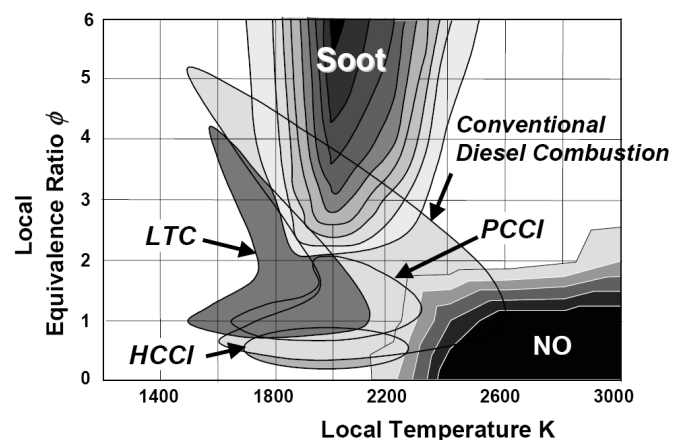


Figure 1 - PCCI, LTC and HCCI concept on a ϕ - T map [1].

As shown in Fig. 1, combustion regimes such as LTC, PCCI and HCCI are associated with combustion processes characterized by lower temperatures and higher local excess air ratio. In such a way, it is possible to remain clear from the region of NO_x and soot production.

The objective is to extend the operating range of non-conventional combustion processes as far as possible on the engine operating domain. The difficulty to manage these kinds of combustions, especially in the high engine speed and high load operating domains, is mainly due to two reasons: from one side, they need an homogeneous mixture whose preparation requires a certain interval of time, and to the other side, as the oxidation process is mostly controlled by chemical kinetics, the combustion control requires the ability to reproduce the most favorable thermodynamic conditions in the cylinder.

In this perspective, new generations of ICE are equipped with different devices, such as EGR loop or CR (*Common Rail*) DI (*Direct Injection*) systems, to perform more flexible engine-system control-strategies. In particular, recent CR injection devices permit the execution of several injections per engine cycle. Consequently, nowadays engine systems present a large number of parameters to set in order to obtain the optimal performances in terms of BSFC (*Brake Specific Fuel Consumption*) and pollutant emissions.

In this context, numerical modeling is becoming a very important tool in industry and academic R&D programs [1-5]. In fact, it permits a large number of numerical tests to be performed in a short interval of time and at reduced costs compared to those associated with experiments. Because of the trade-off between result detail level and CPU cost of computation, in literature it is possible to find different approaches to Diesel combustion modeling. According to the purpose they have, numerical tools can be classified in global-system-simulation adapted-models, requiring a CPU time close to 10^2 the real time, and physical models, most adapted to research purposes, running in about 10^6 the real time. The first class usually includes tabulated-base, empirical and phenomenological models [6-15] while the second includes CFD models [16-23]. In both cases, it is necessary that numerical tool developments follow the technological ones, in order to account for all the phenomena implied.

In the current global system simulation domain, two approaches for direct-injection combustion modeling are predominant in commercial numerical tools (e.g. GT-POWER [24]). On one hand, empirical mathematical models, usually based on the well known Vibe equation [6], are able to greatly reduce the computation time, but prediction accuracy is limited. On the other hand,

phenomenological multi-zone approaches, mostly based on the Hiroyasu et al. approach [15], give a more accurate description of the mixing and the combustion processes; however, in order to have a realistic description of the combustion, the number of zones to be used is often quite large, leading to a significant increase of the CPU time.

The model presented below represents a 0D approach to model Diesel HCCI combustion derived from the reduction of a TKI –PDF (*Tabulated Kinetics for Ignition coupled with PDF*) 3D CFD model developed at the IFP [21,25]. In the following sections, a global overview of the model is given first. Subsequently, the two main parts of the model, the spray and combustion models, are detailed. In the paper, particular attention is paid to the description of the multi-injection modeling. It reveals to be an original approach based on the use of PDFs coupled with tabulated complex-chemistry. Finally, validation of the global combustion model is done by comparing computed results with experimental data. The paper ends with a discussion on model improvements and perspectives.

GLOBAL-MODEL DESCRIPTION

Conventional Diesel and HCCI combustion regimes are governed by different physical mechanisms.

In conventional Diesel combustion, the mixture inside the cylinder is characterized by a high fuel mass fraction stratification. The first site of auto-ignition appears inside the spray, where chemical and thermodynamic conditions are at their most favourable. The most important challenge concerning auto-ignition phase description is to capture the shortest ignition delay. Heat release, due to combustion at the first site, subsequently favours the multiplication of auto-ignition sites. This chain reaction leads to the sharp heat release process typical of the premixed Diesel combustion phase. The remaining fuel burns in a diffusion flame and the heat release is governed by the mixing process. In this phase, turbulence plays the most important role.

In HCCI combustion, the mixture inside the cylinder can be considered as homogeneous. Hence, chemical kinetics plays the most important role in the combustion process. Because of the homogeneity of the mixture, all of the gas auto-ignites simultaneously. As a consequence, HCCI combustion is characterized by a stiff heat release process.

For these reasons, a deep understanding of the spray-formation mechanism is necessary [26-37]. In a general situation, the two combustion regimes are not so well distinguished. Therefore, a modeling challenge is to be able to manage all of the different scenarios. Moreover,

the presence of EGR in the cylinder modifies the chemical kinetics, and phenomena, such as cold flames, could appear at the beginning of the fuel oxidation process. This explains the importance of using a detailed chemical-mechanism. Finally, in the case of multi-injection, all these phenomena must be generalised and integrated into a wider context, in which additional phenomena such as interaction of sprays characterised by different equivalence-ratios and chemical compositions (modified by combustion process) could appear.

In the following approach, in order to overtake the lack of spatial-dimension intrinsic to 0D models, several tools commonly used in 3D modeling have been adapted to a 0D formalism. In particular, the following have been used:

- PDF, to describe the fuel-mass distribution inside the spray,
- tabulated chemistry, to take into account the complex-chemical kinetics,
- κ - ϵ model, to represent the turbulence influence on the mixing process.

Figure 2 shows the synoptical diagram of the global-combustion model in the case of double injection. Directional arrows represent the interactions of the different submodels.

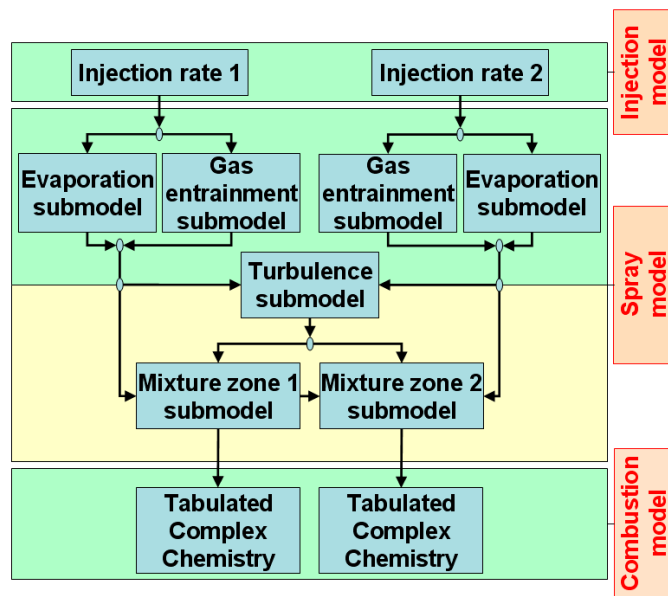


Figure 2 - Synoptical diagram of the complete Diesel HCCI combustion model.

As shown, the global combustion model is made of two main parts:

- the spray model, whose purpose is to represent the formation and the temporal evolution of the spray volume (mixture zone),

- the combustion model, whose role is to compute the heat release and the evolution of the different species characterizing the mixture.

The spray model consists of four different submodels:

- the evaporation submodel, giving the fuel-mass source-term in the spray volume,
- the gas entrainment submodel, giving the ambient-gas (in the most general case considered to be a perfectly stirred mixture of air and EGR) mass source-term,
- the turbulence submodel, computing the turbulence inside the spray; the source terms of the turbulence submodel depend on the fuel and entrained-gas source terms,
- the mixture submodel, describing the fuel-mass distribution inside the spray volume; its source terms are the fuel and entrained-gas mass flow rate inside the spray and the turbulence submodel output, which is directly correlated to the mixing law of the two source terms.

The combustion model consists of a tabulated complex-chemistry inspired by the FPI (*Flame Prolongation of ILDM (Intrinsic Low Dimensional Manifold)*) theory [38-40]. Here, injection rates are supposed to be an input of the model.

In the following, a short description of the different submodels will be given in order to explain the impact they have on the global-combustion model. More attention will be paid in the description of the mixing model, as it represents the major contribution of the paper to the state of the art. Thermal losses have been taken into account by using the well-established theory proposed in [41].

SPRAY MODELING

As shown in Fig. 2, spray model can be decomposed into four submodels that interact with each other.

- The evaporation submodel: it computes the thermodynamic conditions at the liquid-gas interface during the evaporation process, and quantifies the fuel-mass evaporation-rate. It also gives qualitative information concerning the penetration length of the liquid jet of fuel.
- The gas entrainment submodel: it computes the mass of gas entrained in the spray volume. It also gives qualitative information regarding the penetration length of the gaseous spray and an estimate of the spray volume.
- The turbulence submodel: it computes the characteristic frequency associated with the turbulent movement of the gas within the spray.

Turbulent frequency is very important in turbulent combustion, as it is the case in ICE, because it is directly connected to the mixing process of evaporated fuel and entrained gas in the spray volume.

- The mixture submodel: it quantifies the total spray gaseous-mass, and describes the fuel-mass distribution within the spray volume.

EVAPORATION SUBMODEL

The evaporation submodel has two main purposes:

- to compute the thermo-chemical properties, in terms of temperature and composition, of the gaseous mixture at the liquid-gas interface during the liquid-fuel evaporation-process,
- to estimate the overall fuel-mass evaporation-rate within the spray.

Methodology to determine the interfacial properties at the liquid-gas interface has been set up according to the theory proposed in [42]. The theory deals with the steady evaporation-process of a single droplet of liquid, which is supposed to be at rest in a gaseous mixture with given composition, Fig. 3.

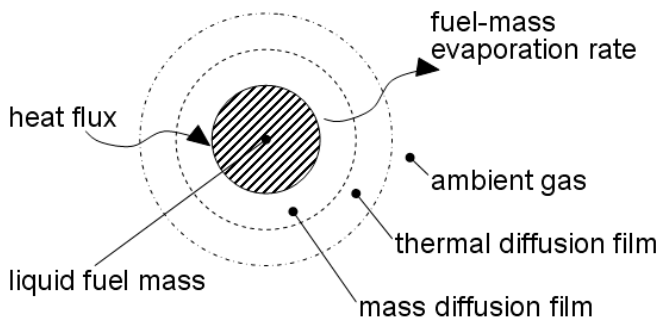


Figure 3 - Evaporation model of a liquid droplet.

Liquid-fuel mass is supposed to have reached its wet-bulb temperature, T_s . Hence, all the heat flux from ambient gas to liquid is used to evaporate the droplet. Moreover, mixture at interface is supposed to be at thermodynamic equilibrium. In such a system, the mass and thermal transfer-processes are respectively characterized by the mass transfer-number, B_m , defined as:

$$B_m = \frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}} \quad (1)$$

where $Y_{F,s}$ and $Y_{F,\infty}$ are respectively the mixture fuel mass-fraction at the interface and ambient-gas conditions, and the thermal transfer-number, B_p , defined as:

$$B_p = \frac{C_{p,g} \cdot (T_\infty - T_s)}{L_{v,s}} \quad (2)$$

where $C_{p,g}$ is the constant-pressure heat-capacity of the mixture at the reference temperature and composition computed using the Sparrow and Gregg 1/3 law according to [42], T_s and T_∞ correspond respectively to the interface and ambient-gas temperature, and $L_{v,s}$ is the fuel latent-heat of vaporization at the interface temperature.

Under the aforesaid hypotheses, the following relation must be verified:

$$B_m = B_p = B \quad (3)$$

The associated equation system is solved iteratively varying the T_s value. More details about the evaporation submodel can be found in [14]. The evaporation submodel allows for the determination of the evaporating liquid-fuel thermo-chemical properties as a function of the pressure, p_∞ , and temperature of the surrounding gas, Fig. 4.

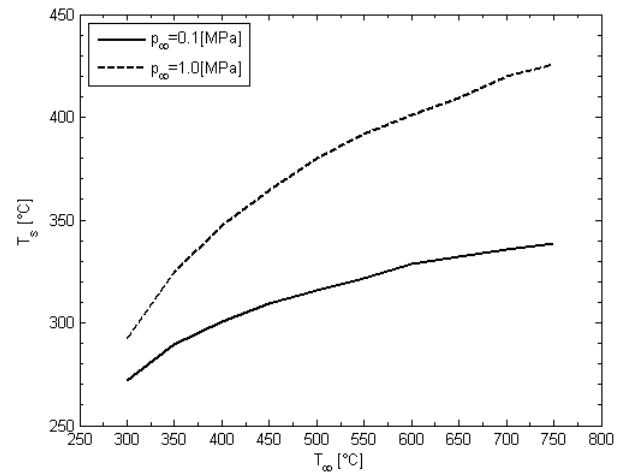


Figure 4 – Influence of the surrounding gas thermodynamic state on the liquid-gas interface temperature for n-heptane [14].

The computed properties at the liquid-gas interface will be used in the mixture characterization submodel and in the combustion submodel presented below. In particular, T_s is very important in spray modeling as it permits an estimate of the local temperature of the mixture.

Concerning the computation of the fuel-mass evaporation-rate, it is worth mentioning that the liquid-fuel mass-distribution within the spray is very complex. In fact, the real scenario consists of droplet-size distribution, ligaments, and undefined geometry of the liquid phase. In a global-system-simulation approach to

solve the associated system of differential equations is not possible because of the CPU cost. For that reason, a more global approach based on the computation of a global characteristic evaporation-time, τ_{ev} , has been preferred.

The overall fuel-mass evaporation-rate, $\dot{m}_F$, is then computed as:

$$\dot{m}_F = C_{ev} \cdot \frac{m_{F,l}}{\tau_{ev}} \quad (4)$$

where C_{ev} is an adjustment constant coefficient of the model, m_F is the mass of gaseous fuel and $m_{F,l}$ represents the liquid-fuel mass.

Characteristic evaporation-time is computed starting from the theory proposed in [29]. This theory permits to estimate the liquid-jet penetration-length, L_o , as a function of the geometry of the injector, the composition of the fluids and their thermodynamic state. τ_{ev} is then computed inverting the equation giving the temporal evolution of the liquid-jet penetration-length, and imposing a liquid penetration equal to L_o . Quantitative results of the model, compared to 3D simulation results relative to ICE application, can be found in [14].

GAS ENTRAINMENT SUBMODEL

This submodel describes the temporal evolution of the spray volumes inside the cylinder and computes the mass transfers between sprays.

Figure 5 shows a 3D computation of the spray-volume evolution in an ICE equipped with a piston bowl with NADI™ (*Narrow Angle Direct Injection*)¹ concept specifications. As can be seen, the narrow angle of injection (angle between the spray penetration and cylinder axes) favours deep penetrations of the spray in the cylinder, (a). Once the tip of the spray impacts the piston, the spray is outward-guided by the bowl shape, (b). Then, the shape of the bowl confers a coherent toroidal movement to the spray, (c)(d). As can be seen, the spray tip reaches the proximity of the injection point before the spray fills up the whole cylinder.

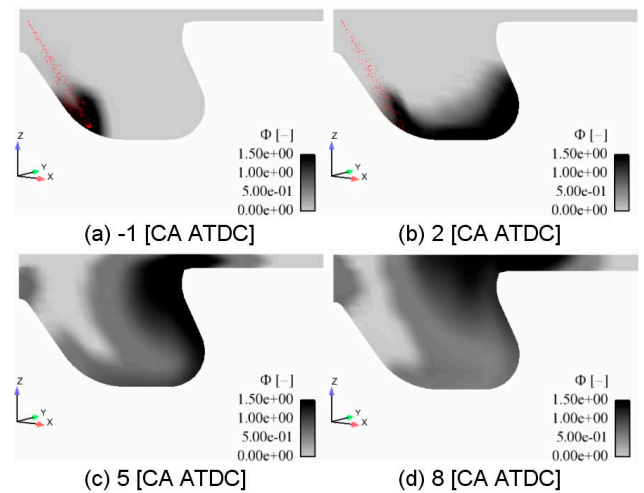


Figure 5 - Typical spray evolution in an ICE equipped with the NADI™ concept specifications. Equivalence-ratio distribution at different crank angle values: -1, 2, 5 and 8 CA ATDC. Engine speed: 1500 rpm.

Here, spray regions are supposed to be perfect truncated cones, Fig. 6. Spray volumes are completely defined once all the penetration lengths, S_p and the spray angles, θ_p are known (subscript i indicating the injection number). The hypothesis that the injection $i+1$ is performed in the spray region of injection i will be retained in the following discussion. This assumption, partially justified by Fig. 5, will be further supported by the good agreement between simulation results and experimental data.

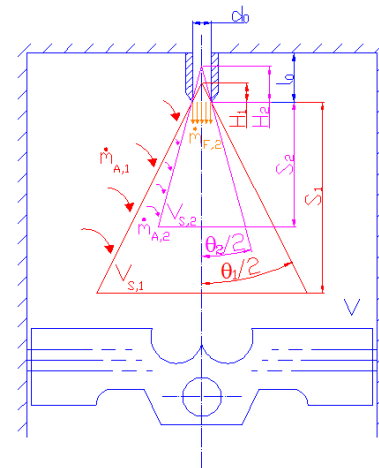


Figure 6 - Description of spray volumes for two injections.

The penetration length of each spray is computed using the well-known semi-empirical correlation given in [26]. According to this theory, once defined the spatial, x_i^* , and temporal, t_i^* , scales as:

¹ All the experimental results presented below refer to an ICE equipped with a piston bowl with NADI™ concept specifications.

$$x_i^+ = \frac{\sqrt{C_a} \cdot d_h \cdot \sqrt{\frac{\rho_{F,l}}{\rho_{A,i}}}}{a \cdot \tan\left(\frac{\theta_i}{2}\right)} \quad \text{and} \quad t_i^+ = \frac{x_i^+}{U_{F,l,i}} \quad (5)$$

where C_a is the orifice coefficient of area-contraction, d_h is the injector hole diameter, ρ_A is the ambient-gas density, $\rho_{F,l}$ is the liquid-fuel density, a is a dimensionless coefficient (authors recommend $a = 0.66$) and $U_{F,l}$ is the fuel velocity in the injector nozzle, penetration length of the i -th spray can be expressed as:

$$S_i = \left[\left(\frac{1}{\frac{t_{inj,i}}{t_i^+}} \right)^q + \left(\frac{1}{\left(\frac{t_{inj,i}}{t_i^+} \right)^{\frac{1}{2}}} \right)^q \right]^{\frac{1}{q}} \cdot x_i^+ \quad (6)$$

and the relative spray opening-angle as:

$$\tan\left(\frac{\theta_i}{2}\right) = C_{\theta,i} \cdot \left[\left(\frac{\rho_{A,i}}{\rho_{F,l}} \right)^{0.19} - 0.0043 \cdot \sqrt{\frac{\rho_{F,l}}{\rho_{A,i}}} \right] \quad (7)$$

where q is a dimensionless coefficient (author recommend $q = 2.2$), $t_{inj,i}$ is the relative-time coordinate referred to injection i with its origin at the SOI (*Start Of the Injection*), and $C_{\theta,i}$ is an adjustment constant-coefficient relative to injection i .

Hence, by using geometrical considerations, the volume of the i -th injection, $V_{S,i}$ is:

$$V_{S,i} = \hat{V}_{S,i} - \hat{V}_{S,(i-1)} \cdot (i > 1) \quad (8)$$

where:

$$\hat{V}_{S,i} = \frac{\pi}{3} \cdot \tan^2\left(\frac{\theta_i}{2}\right) \cdot \left[(S_i + H_i)^3 - H_i^3 \right] \quad (9)$$

is the truncated cone relative to the vapor penetration length of the i -th injection. Definition of H_i can be found in Fig. 6.

This model, relative to a non-reactive single-injection in a constant-volume vessel, has been widely discussed and validated with experimental data [26,27,36]. The model has been shown to be sensitive to variations of parameters such as injection pressure, nozzle geometry and thermodynamic state of vessel ambient-gas. In ICE applications, in-cylinder thermodynamic-conditions vary in time because of the piston motion, thermal fluxes and combustion process. For that reason, in order to take into account the time history of the spray penetrations, the differential form of Eq. (8) has been implemented in the model. As a consequence, spray volume is computed as:

$$V_{S,i} = \int_0^{t_{inj,i}} \dot{V}_{S,i} \cdot dt_{inj,i} \quad (10)$$

This model has been validated for ICE application through comparison of 0D model results with 3D CFD model results in the case of single injection [14].

Spray-volume evolutions determines the entrainment of ambient gas, m_A , in the spray. Hence, for the injection i , the entrained-gas-mass flow-rate is:

$$\frac{dm_{A,i}}{dt} = \rho_{A,(i-1)} \cdot \frac{dV_{S,i}}{dt} \quad (11)$$

In the case of $i=1$, $\rho_{A,0}$ must be considered to be referred to the ambient-gas mixture initially contained in the cylinder.

Figure 7 represents a general case of triple-injection spray evolutions in non-reactive conditions. As shown, although the liquid-fuel injection-rates are all the same for the three injections, (a), the evolutions of the spray volumes are very different from each other because of thermodynamic conditions of the ambient gas and the piston movement, (b). Figure 7 (c) shows the oxygen mass-transfers from one spray to another. As shown, because of the non-reactive conditions, the total initial mass of oxygen is conserved. Finally, the gaseous-fuel mass in the different sprays as well as its global value, are plotted and compared to the liquid-fuel injected-mass, (d).

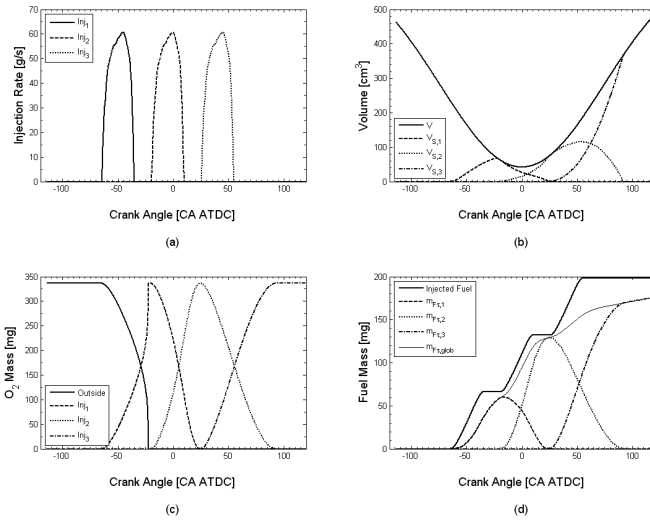


Figure 7 - Triple-injection spray evolutions in non-reactive conditions. Injection rates (a), spray volume evolutions (b), oxygen mass-transfer between sprays (c) and fuel-tracer mass transfer between sprays (d). Global liquid-fuel injected-mass is compared to the global fuel-tracer mass (d).

TURBULENCE SUBMODEL

Turbulence has an enormous impact on the Diesel HCCI combustion process. More particularly, it plays a very important role in the mixture formation process, as it enhances mass, momentum and energy transfer-rates. The goal of the turbulence submodel is to estimate the characteristic turbulent time, τ_t .

The following model is obtained by reduction of the 3D κ - ε turbulence-modeling approach. In the most general way, the balance-equation relative to a closed volume for global kinetic-energy, E_c , can be expressed as the sum of production and dissipation terms:

$$\frac{dE_c}{dt} = \frac{dE_c}{dt} \Big|_{pr} + \frac{dE_c}{dt} \Big|_{ds} \quad (12)$$

According to [43], the spray-associated kinetic-energy represents 98% of the total kinetic energy of the mixture. For that reason all different contributions (e.g. swirl, tumble and squish kinetic energies) will be neglected in what follows.

Hence, the E_c production term can be expressed as:

$$\frac{dE_c}{dt} \Big|_{pr} \cong \frac{dE_c}{dt} \Big|_{spray} = \frac{U_{F,l}^2}{2} \cdot \frac{dm_{F,inj}}{dt} \quad (13)$$

in which:

$$U_{F,l} = \frac{1}{C_d \cdot n_h \cdot \rho_{F,l} \cdot \left(\frac{\pi}{4} \cdot d_h^2 \right)} \cdot \frac{dm_{F,inj}}{dt} \quad (14)$$

where $m_{F,inj}$ is the injected mass of fuel, C_d is the discharge coefficient of the orifice and n_h is the number of injector holes.

By spatially filtering the 3D momentum balance-equation, it is possible to compute the mean specific kinetic-energy, $\tilde{K}^2$:

$$\frac{d\tilde{K}}{dt} = \frac{\sqrt{2 \cdot \tilde{K}}}{m_s} \cdot \left[U_{F,l} \cdot \frac{dm_{F,inj}}{dt} - \sqrt{2 \cdot \tilde{K}} \cdot \left(\frac{dm_A}{dt} + \frac{dm_{F,inj}}{dt} \right) \right] - C_K \cdot \tilde{K}^{N_K} \quad (15)$$

where the last term is an empirical expression representing the closure term relative to the dissipation rate. Here, m_s being the global mass of gases in the spray, and C_K and N_K are two constant coefficients of the model. More details on the derivation of Eq. (15) can be found in [44].

Consequently, the mean specific turbulent-kinetic-energy, $\tilde{\kappa}$, can be computed as:

$$\tilde{\kappa} = \frac{E_c}{m_s} - \tilde{K} \quad (16)$$

The mean specific turbulent-kinetic-energy dissipation-rate, $\tilde{\varepsilon}$, is supposed to have a similar expression to the dissipation-rate term of $\tilde{K}$:

$$\tilde{\varepsilon} = C_\kappa \cdot \tilde{\kappa}^{N_\kappa} \quad (17)$$

where C_κ and N_κ are two constant coefficients of the model.

Equation (12) can now be rewritten as:

$$\frac{dE_c}{dt} = \frac{U_{F,l}^2}{2} \cdot \frac{dm_{F,inj}}{dt} - m_s \cdot (C_K \cdot \tilde{K}^{N_K} + C_\kappa \cdot \tilde{\kappa}^{N_\kappa}) \quad (18)$$

² The symbol tilde means that the variable has been computed using the Favre mean-operator.