DEVELOPMENT OF ADVANCED MODELS FOR COMBUSTION SIMULATIONS IN IC ENGINES

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Abstract
CFD simulation of the combustion process is very important for a correct prediction of both engine performance and pollutant emissions such as soot and NOx. However, combustion modeling involves many complex phenomena that need to be handled in detail. Among them, the most important ones are represented by initial flame kernel formation, flame propagation, fuel oxidation and turbulence-chemistry interaction. Furthermore, the rapid evolution of SI and Diesel combustion systems requires a continuous improvement of the existing numerical and physical models, to correctly account for the effects of stratified or very diluted mixtures, multiple injections and complex fuel kinetics.

In this work, the proposed approaches to model both compression-ignition and spark-ignition combustion are illustrated. In particular, the representative interactive flamelet (RIF) model is used for Diesel combustion. It accounts for both detailed chemistry and turbulence-chemistry interaction. The possibility to use a multiple number of flamelets makes the model also suitable for the simulation of advanced combustion modes including multiple injections. For what concerns SI combustion, the Extended Coherent Flamelet Model (ECFM) is used in combination with a Lagrangian model to describe the first stages of the flame propagation process, where the flame kernel formation and growth processes are influenced also by energy transfer from the spark and heat conduction inside the gas phase.

The proposed set of models has been embedded into the Lib-ICE code, which is a set of libraries and solvers for the simulation of IC engines based on the OpenFOAM® technology. Experimental validation was carried out by simulating spray combustion in a constant-volume vessel and premixed flame propagation in an optical engine.

Diesel spray combustion modeling
Simulation of non-premixed, reacting turbulent flows requires a detailed description of the interaction between turbulence and chemistry, that affects both auto-ignition and mixing-controlled combustion phases. Detailed chemistry is also necessary to account for the complex fuel oxidation process under a wide range of operating conditions (temperature, pressure, equivalence ratio and residual gas fraction). Among the different proposed approaches, flamelet models are widely
used. Their main assumption is that both auto-ignition and combustion of a turbulent diffusion flame can be predicted by solving the reaction-diffusion problem in the mixture fraction space for an equivalent igniting laminar diffusion flame, where effects of turbulence and flow field are taken into account by means of the scalar dissipation rate [1].

To better describe the flame structure, the possibility to use a multiple number of flamelets was also introduced [2,3]. In particular, each flamelet represents a certain portion of the injected fuel mass and evolves independently with its own scalar dissipation rate. In this way, effects of flow field are better accounted for, with the possibility to predict local flame extinction close to the nozzle, where gas velocities and mixture fraction gradients are very high. In the proposed approach, for each flamelet, the reaction diffusion problem is solved for both chemical species and sensible enthalpy assuming unit Lewis number. Equations are solved on a 1D mesh representing the mixture fraction space. To reduce the computational time and allow the use of detailed chemistry, the TDAC algorithm was also employed to limit the operation of the ODE stiff solver when chemistry has to be integrated [4]. The chemical composition in each computational cell is computed from flamelet species profiles in the mixture fraction space and flamelet marker functions $I$:

$$\tilde{Y}_i(x) = \sum_{j=1}^{N_f} I_j(x) \cdot \int_0^1 Y_j(Z) p(Z) dZ$$

where $Z$ is the mixture fraction and $p(Z)$ is assumed to be a $\beta$-pdf, whose coefficients are computed in each cell from mixture fraction and its variance $Z'^2$.

Figure 1 illustrates the code structure employed to simulate diesel combustion in Lib-ICE, with emphasis on the information exchange between the CFD solver and the flamelet library.

Simulations of diesel spray combustion at constant-volume vessel were carried out using n-heptane as fuel with experimental data provided by the Engine Combustion Network database (http://www.ca.sandia.gov/ecn). Different operating conditions
were simulated including variations of ambient density, temperature and oxygen concentration. The spray evolution is modeled by the Lagrangian approach, and details about the sub-models employed can be found in [5]. During the simulation, the grid was dynamically refined in regions where the fuel-air mixing process takes place, to increase the simulation accuracy and contemporary reduce both grid dependency and CPU time. The spray model was validated at non-reacting conditions and Figure 2 provides a comprehensive comparison between computed and experimental data in terms of liquid and vapor penetration (Fig. 2a), radial mixture fraction profiles at different distances from the injector (Fig. 2b) and fuel vapor distribution at 0.9 ms (Fig. 2c). A correct prediction of the fuel vapor inside the chamber is very important since it significantly affects the scalar dissipation rate distribution that is then used by the combustion model.

**Figure 2.** Comprehensive spray model validation. Comparison between computed and experimental data of: (a) liquid and vapor penetration; (b) radial mixture fractions profiles at different distances from the injector; (c) fuel vapor distribution at 0.9 ms. Operating condition: non-reacting (0% O₂); \( ρ_{\text{amb}} = 14.8 \); \( T_{\text{amb}} = 1000 \) K.

Once the spray model was completely assessed, simulations at reacting conditions were carried out using the reduced mechanism for n-heptane proposed by Lu and Law [6]. Each case simulates the first two milliseconds of injection time using 40 flamelets, each one of them representing 5% of the injected fuel mass.

Fig. 3 displays the validation of the combustion model. In particular, Fig. 3(a) compares computed and experimental data of ignition delays for different ambient oxygen concentrations and at two different ambient densities. The experimental trend is rather well described by the model at 14.8 kg/m³ density. Results are still rather satisfactory also at 30 kg/m³, where the computed overestimation is both related to the kinetic mechanism and the spray model that was not validated at such density. The dependency of the ignition delay on the ambient temperature is rather well reproduced as shown in Fig. 3(b), the underestimation at 1300 K is acceptable and probably due to the kinetic mechanism used. Finally, in Fig. 3(c) computed and experimental pressure derivatives versus time are compared for three different ambient oxygen concentrations. The proposed combustion model is able to reproduce both the parts of the Diesel combustion process (auto-ignition and
mixing controlled combustion) with an acceptable agreement with experimental data. Future work on Diesel combustion modeling is necessary to improve the prediction of the flame structure in order to correctly predict both the lift-off length and soot distribution.

**Figure 3.** Validation of the multiple representative interactive flamelet model: (a) effects of oxygen concentration on ignition delay at two different ambient density values (14.8 kg/m$^3$ and 30 kg/m$^3$); (b) effects of ambient temperature at 14.8 kg/m$^3$ density; (c) comparison between computed and experimental vessel pressure derivative versus time for three different ambient oxygen concentrations (10%, 12%, 15%, 21%) at 14.8 kg/m$^3$ density.

**Spark-ignition combustion modeling**

SI engine combustion is influenced by different phenomena such as electrical circuit properties, local flow conditions, turbulence intensity and fuel vapour distribution inside the combustion chamber. Hence, the initial formation and evolution of the flame kernel need to be described in detail, since it will determine the subsequent turbulent flame propagation process and the cylinder pressure history. In the proposed model, the spark-channel is represented by a set of lagrangian particles, that are initially placed along a line between the two electrodes. Particles are convected by the mean flow and, for all of them, equations of mass and energy are solved. In these equations both the local laminar flame speed and the heat transferred from the electrical circuit through the spark electrodes are taken into account. Specific sub-models estimate the instantaneous amount of energy transferred from the secondary circuit to the gas phase and calculate the flame kernel expansion velocity accordingly, taking also the real properties of the high-temperature gas into account. At each time-step, the flame surface density distribution is reconstructed once particle positions and their radius are known. Such quantity is then used by the combustion model to calculate the fuel burning rate. Details of the employed sub-models are displayed in Fig. 4. The flame kernel model is de-activated once a turbulent flame structure is established. At that time, the Extended Coherent Flamelet Model [7] is used in the remainder of the simulation.
Figure 4. Overview of the features of the main sub-models used to predict flame kernel evolution in SI engines: (a) calculation of flame surface density $\Sigma$ from distribution and size of particles; (b) electrical circuit sub-model; (c) model to describe the plasma channel expansion due to energy transfer from the electrical circuit.

Experimental validation of the model was performed by simulating the experiments carried out by Herveg and Maly in an optical engine with a combustion prechamber [8], where different engine speeds, air/fuel ratio, ignition systems and spark-plug positions were tested: details of the simulated domain are displayed in Fig. 5(a), together with the predicted velocity field in Fig. 5(b). The computed evolutions of the gas velocity and turbulence intensity in the periphery of the combustion chamber are compared with LDV measured data in Fig. 5(c). An acceptable agreement was achieved, making possible to proceed with combustion simulations.

Figure 5. Details of the simulated optical engine: (a) cylinder geometry with combustion pre-chamber; (b) computed velocity field at TDC; (c) comparison between computed and experimental evolution of velocity and turbulence intensity values.

Results of combustion simulations are summarized in Fig. 6, where computed and experimental evolutions of in-cylinder burned volumes are compared. The proposed model for SI combustion reproduces quite well the dependency of the burned volume evolution as function of the equivalence ratio and engine speed for the case where the spark is centrally located in the combustion chamber (see Figs.
6(a)-(b)). For what regards the conditions in which the spark-plug is peripherally mounted, the computed burned gas region is in agreement with experimental images acquired by Schlieren photography, as shown in Fig. 6(c). Achieved results are rather promising and future work will be mainly focused on the extension of this model for the prediction of stratified combustion and soot emissions in GDI engines.

Figure 6. SI combustion model validation: (a) effects of the relative air/fuel ratio; (b) effects of the engine speed; (c) comparison between computed and experimental optical burned gas regions.

References


