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Modeling diesel combustion with tabulated kinetics and different flame structure assumptions based on flamelet approach

Tommaso Lucchini1, Daniel Pontoni1, Gianluca D’Errico1 and Bart Somers2

Abstract
Computational fluid dynamics analysis represents a useful approach to design and develop new engine concepts and investigate advanced combustion modes. Large chemical mechanisms are required for a correct description of the combustion process, especially for the prediction of pollutant emissions. Tabulated chemistry models allow to reduce significantly the computational cost, maintaining a good accuracy. In the present work, an investigation of tabulated approaches, based on flamelet assumptions, is carried out to simulate turbulent Diesel combustion in the Spray A framework. The Approximated Diffusion Flamelet is tested under different ambient conditions and compared with Flamelet Generated Manifold, and both models are validated with Engine Combustion Network experimental data. Flame structure, combustion process and soot formation were analyzed in this work. Computed results confirm the impact of the turbulent–chemistry interaction on the ignition event. Therefore, a new look-up table concept Five-Dimensional-Flamelet Generated Manifold, that accounts for an additional dimension (strain rate), has been developed and tested, giving promising results.

Keywords
Computational fluid dynamics, combustion modeling, diesel, Approximated Diffusion Flamelet, Flamelet Generated Manifold, Five-Dimensional-Flamelet Generated Manifold, Spray A

Introduction
The continuous development of the existing technology of compression ignition engines requires a deep knowledge of the complex thermal, chemical and fluid dynamics processes that govern the combustion process to further improve its efficiency and quality of exhaust gases.1–4 Novel advanced combustion systems as well as optimal chamber design and fuel injection strategies5,6 and more efficient after-treatment devices (SCR, LNT, DPF, DOC)7–10 are required to meet the more and more stringent regulations.11 Moreover, potentialities associated with the use alternative fuels, eventually mixed with the conventional ones, must be well assessed.12–15 To this end, it is necessary to perform both fundamental and applied studies by means of advanced numerical and computational techniques. The Engine Combustion Network (ECN)16 has been built over the last decade supported by this motivation: the creation and availability of large databases with high-quality experimental results generated at different international institutions to deep the fundamental understanding of the injection and combustion process and support the validation and development of computational fluid dynamics (CFD) combustion models.17 Focusing on Diesel combustion, a large number of experiments were carried on not only by injecting n-dodecane sprays, chosen as Diesel fuel surrogate, in a

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constant-volume vessel chamber, recording ignition delays (IDs) and pressure rise (and hence the rate of heat release rates), but also collecting quantitative information about the flame structure, such as lift-off lengths (LOLs) and soot distributions.

Open discussion in the ECN community evidenced the importance of a detailed chemical mechanism to be employed in the CFD approach to correctly estimate both global combustion parameters and details of transient flame structure. However, the Direct integration of chemistry equations to compute reaction rates is computationally demanding since it involves a large number of species and the use of ordinary differential equation (ODE) stiff solvers. For this reason, the size of the chemical mechanism which can be used in practical simulations is limited both in terms of species and reactions. An interesting alternative for the reduction of CPU time is the tabulated kinetic approach, in which the reaction rates are stored in a look-up table and retrieved during the simulation, as a function of the thermodynamic state of the system. The combustion models can then also include the effect of turbulence-chemistry interaction, for a better prediction of ignition and combustion of Diesel spray. To this aim, the flamelet approach is widely accepted where chemical reactions are assumed to take place in an ensemble of small laminar flames also called flamelets. Objective of this work is to compare two approaches which are both based on the flamelet assumption and make use of tabulated kinetics. The first is called Approximated Diffusion Flamelet (ADF) while the second is the Flamelet Generated Manifold (FGM). Both the approaches are analyzed in terms of their capability to predict auto-ignition and flame stabilization process. ADF approach is based on approximated flamelets, which are computed by employing the Homogeneous Reactor table. FGM model consists of storing and retrieving low-dimensional manifolds created using solutions of one-dimensional diffusive flames with direct integration of detailed kinetic chemistry, by means of the CHEM1D application: the thermal state of a reacting spray is expressed as function of four variables: pressure, ambient temperature, mixture fraction and progress variable. An extension of this approach, which was also tested in the current investigation, consists in a novel model, called Five-Dimensional-Flamelet Generated Manifold (5D-FGM): the additional dimension of the table is the applied strain rate. A better description of the whole combustion process was achieved, especially for the low reactivity cases, emphasizing the importance of turbulence-chemistry interaction for a correct prediction of ignition and flame stabilization.

**Computational model**

Diesel combustion is affected by the complex interplay between turbulence and chemistry which determines the auto-ignition time, heat release rate during mixing controlled combustion and the distance from the nozzle at which the flame stabilizes (LOL). Different approaches to couple turbulence and chemistry were proposed in the past and they can be mainly classified in the way chemical kinetics and turbulence-chemistry interaction are handled. For what regards the computation of the chemical species reaction rates, it is important to note that the two possible solutions are either to use direct integration or to generate an offline look-up table. Despite the fact that the first approach is surely more detailed and flexible, it is also computationally very demanding due to the necessity of employing stiff solvers with very small time-steps to estimate the chemical species reaction rates. This aspect introduces several limitations for the maximum number of species that can be used in practical simulations and the consequent accuracy of the adopted mechanism. Moreover, accounting for sub-grid mixing and turbulence-chemistry interaction introduces further computational overheads. This is related to the integration of the presumed probability function, or the transport of many species and energy equations such as the number of simulated flow realizations or stochastic fields. Therefore, tabulated kinetics can offer a possible solution to reduce the CPU time and to keep an acceptable accuracy. Reaction rates and chemical composition are stored in a look-up table which is generated from a chemical mechanism and the assumption of a certain flame structure like a well-stirred reactor or laminar diffusion flame.

Figure 1 illustrates how the CFD solvers based on tabulated kinetics work. Additional transport equations are solved with the Reynolds-averaged Navier–Stokes (RANS) method for mixture fraction $Z$, mixture fraction variance $Z^2$, progress variable $\tilde{C}$ and unburned gas enthalpy $\tilde{h}_u$ which is then used to estimate the corresponding unburned gas temperature $T_u$. In case diffusion-mixing effects are considered, the stoichiometric scalar dissipation rate $\tilde{\chi}_d$ is also computed. The look-up table is accessed with local cell values of $Z$, $\tilde{h}$ and $\tilde{\chi}_d$. This equation is then used to estimate the corresponding heat release rate $\langle h \rangle$.
$Z^2, \tilde{C}, \tilde{\rho}, T_u$ and $\tilde{\chi}_u$, and it provides the chemical composition and the progress variable reaction rate to the solver.

Two different combustion models based on tabulated kinetics were employed in this work: their corresponding look-up tables are generated from laminar diffusion flamelet calculations. The models will be referred as ADF and FGM.

The main difference between ADF and FGM is related to the way reaction rates are estimated during the table generation process. In the ADF case, they are in turn taken from a look-up table based on homogenous auto-ignition calculations. Reaction rates are directly computed using detailed kinetics in the FGM table generation.

**ADF table**

Purpose of the ADF model is to provide a realistic description of the turbulent diffusion flamelet: it takes into account turbulence-chemistry interaction, sub-grid mixing and premixed propagation, thanks to the scalar dissipation rate $\chi$, which controls the diffusion rate of the species.\(^{19,21}\) Flamelet equations are solved in the mixture fraction space in an approximate way, only for the progress variable and the enthalpy, assuming unity Lewis number\(^{22}\)

\[
\begin{align*}
\frac{\partial C}{\partial t} &= \rho \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial z} \right) + \dot{C} \\
\frac{\partial h}{\partial t} &= \rho \frac{\partial}{\partial z} \left( \frac{\partial h}{\partial z} \right) + \frac{\partial \rho}{\partial t}
\end{align*}
\]

where $C$ is the progress variable, defined as the heat release by the combustion.\(^{19,22}\) The progress variable source term $\dot{C}$ is taken from a look-up table which is generated from homogeneous reactor auto-ignition calculations.\(^{19}\) To avoid too anticipated ignitions related to progress variable diffusion, the progress variable reaction rate is set to zero when the equivalence ratio $\phi$ is higher than 3. ADF table is generated according to user-defined mixture fraction variance segregation factors $S_Z$. Subsequently, the scalar dissipation rate $\chi$, for equations (1) and (2), is computed according to Peters’ model\(^{32}\)

\[
\chi = \chi_u \frac{\exp(-2[\text{erfc}^{-1}(2\tilde{Z})]^2)}{\exp(-2[\text{erfc}^{-1}(2Z_{\text{eq}})]^2)}
\]

To account for the sub-grid mixing, a $\beta$-distribution is assumed for both the chemical composition and the progress variable: the corresponding values at user-specified mixture fraction table points are

\[
f\left( t, \tilde{Z}, Z^{m^2} \right) = \int_{0}^{Z} f(z, t) P(z, \tilde{Z}, Z^{m^2}) dz
\]

\[Z^{m^2} = S_Z(1 - \tilde{Z})\]  

where $Z^{m^2}$ values are computed from the corresponding user-defined mixture fraction variance segregation factors $S_Z$ to avoid numerical integration errors which might negatively affect the model consistency in terms of energy conservation; in case of very low variances, the $\beta$-distribution is approximated with a $\delta$-distribution.

A small time-step is necessary during the ADF table generation process to correctly account for the combined effects of mixing and reaction (Figure 2). ADF table should be generated with a large enough range of $\chi_u$ to include extinction, allowing a correct description of the diffusion flame stabilization process.

Solving the flamelet equations with tabulated kinetics introduces an approximation with respect to the case where detailed chemistry is used. To this end, authors have performed in Lucchini et al.\(^{18}\) constant-volume vessel spray combustion calculations with the representative interactive flamelet model using a single flamelet with both detailed and tabulated kinetics. Similar results were found for both the approaches, with the largest difference noticed for conditions of low ambient oxygen concentration.

**FGM table**

Unsteady counter-flow diffusion flame calculations with detailed kinetics are conveniently processed for the generation of the FGM look-up table (Figure 3). Computed results are parameterized as function of the mixture fraction $Z$ and the progress variable $c$: a low-dimensional manifold is generated considering the solution of unsteady one-dimensional flamelet equations in the physical space.\(^{28,29,33}\)
\[
\frac{\partial p}{\partial t} + \frac{\partial p u}{\partial s} = - \rho K
\]  
\[(6)\]

\[
\frac{\partial p Y_i}{\partial t} + \frac{\partial p u Y_i}{\partial s} = - \rho K Y_i + \frac{\partial}{\partial s} \left( \rho D \frac{\partial Y_i}{\partial s} \right) + \dot{\omega}_i
\]  
\[(7)\]

\[
\frac{\partial h}{\partial t} + \frac{\partial p u h}{\partial s} = - \rho K h + \frac{\partial}{\partial s} \left( \lambda \frac{\partial h}{\partial s} + \frac{\partial P}{\partial s} \right)
\]  
\[(8)\]

where \(s\) is the spatial coordinate perpendicular to the flame front, \(D\) is the diffusion coefficient and \(K\) is the flame stretch rate. This last variable has a large influence on the mass burning rate: it is defined as the relative rate change of mass contained in the infinitesimal volume:

\[
K = \frac{1}{M} \frac{dM}{dt}
\]  
\[(9)\]

The flamelet stretch field \(K\) is computed from the transverse momentum equation

\[
\frac{\partial p u K}{\partial x} = \frac{\partial}{\partial x} \left( \mu \frac{\partial K}{\partial x} \right) - 2\rho K^2 + \rho_0 a^2
\]  
\[(10)\]

\(a\) denotes the applied strain rate at the oxidizer side and it is related to the velocity gradient. Equations (6)–(8) are solved by means of the CHEM1D tool. The user specifies the boundary conditions, namely \(T_u, T_{fuel}, p, a\), air and fuel composition. Computed results are post-processed and stored in a look-up table by means of a MATLAB script.

The progress variable source term and the chemical composition are determined as a function of \(c\). Differently from the ADF model, the progress variable is defined as a linear combination of chemical species, which are assumed to be able to describe the whole combustion process, from ignition, low- and high-temperature heat release phases and eventually the fully established diffusion flame

\[
C = 2.70 Y_{H_2O} + 1.50 Y_{CH_2O} + 0.9 Y_{CO} + 1.20 Y_{H_2O} + 1.20 Y_{CO_2}
\]  
\[(11)\]

The FGM table is generated by post-processing the results provided by CHEM1D simulations. During such stage, the user specifies the table discretization in terms of mixture fraction \(Z\) and progress variable \(c\). The FGM combustion model considers only one strain rate and it does not account for sub-grid mixing for the estimation of the chemical composition in the computational cells.

### 5D-FGM table

The 5D-FGM is a new concept developed in the context of this work with the main purpose to improve the prediction of the ID and flame stabilization process. The 5D-FGM table is generated by processing results of flamelet computations with multiple strain rates performed with CHEM1D. To be used in the CFD solver, the strain rate is converted into the stoichiometric scalar dissipation rate by means of Peters’ model:

\[
\chi_{st} = \frac{a}{\pi} \exp \left[ -2(\text{erfc}^{-1}(2Z_{st}))^2 \right]
\]  
\[(12)\]

The MATLAB script is employed for post-processing the flamelets. Accordingly, the table grows of one dimension, as reported in the variable hierarchy map, Figure 4.

### Experimental validation

The Spray A experiment, which was widely studied in the context of the ECN, was used to validate the proposed combustion models. \(n\)-Dodecane fuel is delivered through a single-hole nozzle in a constant-volume vessel with a cubic shape where optical accessibility is ensured by sapphire windows. Different measurement techniques allow to gather information regarding the flame structure, heat release rate, LOL and soot distribution. Simulations were carried out in a two-dimensional computational mesh with the RANS technique. The average mesh size was 0.5 mm which was further reduced to 0.2 mm in the nozzle region. In all the simulated operating conditions, the injection pressure and duration were set to 150 MPa and 5.5 ms, respectively. The injection profile of the 210370 nozzle was used in CFD simulation. \(n\)-Dodecane oxidation chemistry is modeled using the mechanism proposed by Yao et al., which includes 54 species and 269 reactions. Table 1 reports the main details of the simulated
operating conditions: different ambient temperatures and oxygen concentrations were considered when keeping the vessel density to a constant value of 22.8 kg/m$^3$.

A summary of the applied sub-models for Spray A simulation, turbulence and soot assessment is illustrated in Table 2.

Simulations were carried out using the standard $k$–$\epsilon$ turbulence model with the round jet correction ($C_1 = 1.5$). For assessment of spray and turbulence models, non-reacting conditions were first considered with the same ambient temperature of 900 K used in the so-called baseline condition. Figure 5 shows that computed vapor penetration results are in rather good agreement with experimental data. Such result is a fundamental prerequisite for a successful simulation of the combustion process. Further validation under non-reacting conditions was reported in D’Errico et al.\textsuperscript{22}

Four chemistry tables have been generated, one for each analyzed oxygen concentration, Table 3 reports the discretization which represents a good tradeoff between accuracy, computational time and memory consumption. The stoichiometric scalar dissipation rate values follow a logarithmic curve and any further increase in $x_{st}$ resolution does not significantly improve the quality of the results.

For what regards the FGM combustion model setup, since the simulation of the flamelet is very time-consuming (direct integration of the chemistry), and to avoid computational memory issues, a lower number of discretization points in temperature and pressure have been selected, and the applied strain rate has been assumed to a fixed value equal to 700 s$^{-1}$ (Table 4). In previous studies, such value was generally found close to the LOL.\textsuperscript{38,39}

The baseline condition ($O_2 = 15\%$, $T = 900$ K and $\rho_{amb} = 22.8$ kg/m$^3$) was first considered to analyze ADF and FGM results. In particular, Figure 6 compares the computed heat release rate (RoHR) with the apparent experimental value. Heat losses were not included in CFD simulations and this is the reason why the computed data overestimate the experimental ones. Figure 6 illustrates that both ADF and FGM models correctly describe the main features of the Diesel combustion process.

Three events can be clearly detected:

- Ignition, corresponding to the RoHR peak;
- Mixing controlled combustion phase, where RoHR reaches an almost stable value;
- Burnout, corresponding with the drop of RoHR.

The ADF model better predicts the ID time, heat release rate transition from auto-ignition to mixing

<table>
<thead>
<tr>
<th>Table 1. Simulated conditions for ECN Spray A.</th>
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<tbody>
<tr>
<td>Case</td>
</tr>
<tr>
<td>Baseline</td>
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<tr>
<td>Low-T</td>
</tr>
<tr>
<td>High-T</td>
</tr>
<tr>
<td>$O_2$-13</td>
</tr>
<tr>
<td>$O_2$-21</td>
</tr>
<tr>
<td>Non-reacting</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2. Sub-models used on diesel spray simulations.</th>
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</thead>
<tbody>
<tr>
<td>Phenomenon</td>
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<tr>
<td>Turbulence</td>
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<tr>
<td>Spray evolution</td>
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<tr>
<td>Spray breakup</td>
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<tr>
<td>Droplet heat transfer</td>
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<tr>
<td>Evaporation</td>
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<tr>
<td>Scalar dissipation rate</td>
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<tr>
<td>Soot</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3. ADF table discretization.</th>
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</thead>
<tbody>
<tr>
<td>Variable</td>
</tr>
<tr>
<td>Temperature (K)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Mixture fraction (–)</td>
</tr>
<tr>
<td>Normalized progress variable (–)</td>
</tr>
<tr>
<td>Stoichiometric scalar Dissipation rate (s$^{-1}$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 4. FGM table discretization.</th>
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</thead>
<tbody>
<tr>
<td>Variable</td>
</tr>
<tr>
<td>Temperature (K)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Mixture fraction (–)</td>
</tr>
<tr>
<td>Normalized progress variable (–)</td>
</tr>
</tbody>
</table>
controlled combustion and duration of the burnout phase. This aspect is probably related to the fact the ADF includes the effects of sub-grid mixing. Figure 7(a) and (b) compares the FGM and ADF models during the auto-ignition process in the temperature-mixture fraction plane. Time evolution of the most reactive mixture fraction conditions is illustrated with the black line while the red circles show temperature-mixture fraction scatter plot after auto-ignition. For both the models, the ignition is predicted at the side interface between spray and ambient air, and then the kernel moves burning the premixed fuel underneath. However, in FGM, the intermediate temperature reactions occur at richer mixture fraction location (as depicted in Figure 7(b)). To avoid a too anticipated ID, in all the ADF simulations, the reaction rate was set to zero for $\phi > 3$ and this is the reason why temperature clearly drops down at $Z_{\text{max}} = 0.124$ in Figure 7(a).

FGM and ADF flame structures are compared in terms of scatter plots of OH, formaldehyde and acetylene mass fraction as function of $Z$. The magnitude of $Y_{\text{CH}_2\text{O}}$ between the two combustion models is similar, but the location of the peak is different, more toward rich mixture (near the injector) in case of FGM as shown in Figure 8(a). The main reason is the limitation of progress variable source term in case of ADF. Both models predict a correct location of the OH peak close to the stoichiometric mixture fraction value. However, inclusion of sub-grid mixing via mixture fraction variance is probably the reason for a lower maximum OH value for ADF combined with a larger portion of the mixture fraction space where OH was found. A similar behavior can also be found for the $C_2H_2$ mass fraction as it can be seen from Figure 8(c).

Flame LOL and ID time were selected as combustion indicators for the validation of the proposed combustion models under the selected operating conditions reported in Table 1. Following ECN definitions, the LOL is computed as the axial distance between injector orifice and the first location where Favre-average OH mass fraction reaches 14% of its maximum in CFD domain; the ID time is identified by the instant where maximum temperature rise rate reaches the highest value. Effect of ambient temperature on ID and LOL is presented in Figure 9. The ADF model is not fully capable to provide good representation of LOL, especially at low temperature. Shorter value computed with ADF seems to be related to the diffusion of the progress variable leading to a faster stabilization: a possible reason for such discrepancy might be related either to the use of approximate flamelet equations in the table generation process or in the progress variable definition. Predicted LOL is very important for the computed soot distribution since it determines the
amount of rich mixture which burns producing soot precursors.

Effects of oxygen concentration on combustion indicators are reported in Figure 10. Both the models correctly predict an increase of LOL and ID time when reducing the O₂ concentration at 900 K ambient temperature. Computed ID times from the ADF combustion model are in better agreement with experimental data while the LOL is slightly underestimated.

Results from Figures 9 and 10 illustrate that the ADF model better estimates the ID compared to FGM probably because it accounts for mixing effects via $x_{st}$.

A correct prediction of ID is rather important, mainly in the case of engine operation under kinetically controlled combustion modes such as premixed charge compression ignition (PCCI) and reactivity controlled compression ignition (RCCI).

To investigate how stoichiometric scalar dissipation rate affects the auto-ignition process, in Figure 11, the state of mixing $Z^2$ and reaction progress $c$ was reported as function of the stoichiometric scalar dissipation rate $x_{st}$ before auto-ignition for all the cells with $\phi = 2$ which was identified as the most reactive equivalence ratio. Two different ambient temperatures, 850 and 1000 K, were investigated. Ignition is possible only at low $x_{st}$ due to the lower mixture reactivity in the 850 K ambient temperature condition: the maximum progress variable is found in the stoichiometric scalar

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**Figure 8.** Comparison between FGM and ADF models using scatter plots of the most important chemical species used to describe the combustion process: (a) CH₂O, (b) OH (b) and (c) C₂H₂. Results are reported at 4 ms after start of injection.

**Figure 9.** LOL and ID comparison between ADF, FGM and experimental data for different initial conditions of unburned gas temperature with 15% O₂ concentration.
dissipation rate range of 0–10 and then it decreases to zero. For this reason, ignition is expected to take place at the periphery of the jet. Reaction rate increases with ambient temperature and this is the reason why at the 1000 K condition it is possible to find non-zero progress variable values also in the 10–100 range of $X_{st}$ and the ignition spots are located closer to the nozzle. This investigation shows the importance of strain rate inclusion in the combustion model for a correct prediction of the ID.

5D-FGM

The 5D-FGM model was tested over the same conditions presented in Table 1. Inclusion of the strain rate effects is expected to improve the ID predictions. The tabulated strain rate interval, following a logarithmic profile, is displayed in Table 5.

The inclusion of the strain rate effects improves the predictive capability of the 5D-FGM model. Figures 12 and 13 illustrate that IDs are better estimated for the low reactivity conditions ($T_{amb} = 850, 900 \text{ K}$; $O_2 = 13\%, 15\%$) where chemical reactions mainly take place in presence of low strain rates. No significant improvements are reported for the prediction of the LOL, since it is mainly affected by high strain rate close to the nozzle and a reasonable value was already used for the generation of the FGM table. On the other hand, the high reactivity cases

---

Table 5. SD-FGM table discretization.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Number of points</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strain rate (s⁻¹)</td>
<td>8</td>
<td>100–2000</td>
</tr>
</tbody>
</table>

---

Figure 10. LOL and ID comparison between ADF, FGM and experimental data at constant ambient temperature (900 K) and different O₂ concentrations.

Figure 11. Effects of mixing and turbulence for the most reactive cells right before ignition. Progress variable and mixture fraction variance are reported as function of the stoichiometric scalar dissipation rate. The most reactive equivalence ratio is assumed to be equal to 2.

Figure 12. ID and LOL comparison between FGM and 5D-FGM, for different ambient temperatures.

Figure 13. ID and LOL comparison between FGM and 5D-FGM, for different oxygen concentrations.
(1000 K and 21%) are weakly affected, mainly because they sustain ignition and burning phases at higher $\chi_{\text{in}}$, near the nozzle: the experimental LOL is small for the high reactivity case, indeed. The LOL is not strongly influenced, comparing FGM and 5D-FGM, and the trend remains close to the experimental curve.

Only the 13% oxygen case shows the highest difference in terms of LOL. To investigate the reason for such variation, the combustion efficiency was analyzed in Figures 14 and 15. The experimental lower heating value (LHV) of n-dodecane was compared with the one resulting from the ratio between cumulative heat release and injected fuel mass in the FGM and 5D-FGM simulations. To respect the energy conservation, the estimated LHV must be as much close as possible to the experimental value. 5D-FGM better fulfills the energy conservation requirement with respect to the standard FGM model: the use of a single strain rate is the main reason for the underestimation of heat release during the end of combustion phase. The improvement is significant mainly for the $\text{O}_2 = 13\%$ condition and this also explains the reason for a predicted shorter LOL. For the sake of completeness, the same efficiency analysis has been carried out for the ADF simulations: all the simulated points have a combustion efficiency higher than 99.50%.

### Soot prediction of ADF model

The capability of the proposed combustion approach for soot prediction was investigated thanks to the availability of soot volume fraction ($f_v$) maps achieved by means of the diffused back illumination (DBI) technique. The current FGM model implementation does not include the soot model and for this reason, only ADF results are shown in this section. Authors expect that they can also be representative of what could be predicted by the FGM model, since both the approaches estimate similar species distribution, ID

![Figure 14. Cumulative RoHR comparison between FGM, 5D-FGM and LHV of n-dodecane, for different ambient temperatures.](image)

![Figure 15. Cumulative RoHR comparison between FGM, 5D-FGM and LHV of n-dodecane, for different oxygen concentrations.](image)

![Figure 16. Soot assessment for the baseline condition ($\text{O}_2 = 15\%$, $\rho_{\text{amb}} = 22.8 \text{ kg/m}^3$): (a) soot mass evolution in time and (b) soot fraction volume location and concentration at $t = 4 \text{ ms}$.](image)
times and LOL values. Tuning of the Leung-Lindstedt and Jones (LLJ) model was carried out for the baseline condition including also the contribution of O and OH to soot oxidation.\cite{41,42} Figure 16(a) shows the cumulative soot mass within the optical window for the baseline condition (O$_2$ = 15%, $\rho_{amb}$ = 22.8 kg/m$^3$). The onset of soot production is well predicted, but the slope of the curve during the inception interval is lower in the CFD model. The soot mass peak is underestimated in magnitude, but the time when it occurs is fairly captured. The steady-state value is correctly estimated, as the time and slope of the curve during the complete oxidation of soot particles. Figure 16(b) shows that the soot volume fraction distribution is rather well described by the ADF model. Such results are not only due to a correct selection of the LLJ model constants, but also due to a correct estimation of the flame LOL.

Figure 17 reports the evolution of the soot mass as a function of time for the three different ambient temperatures $T_{amb}$ at 15% ambient oxygen concentration. The model is capable to reproduce the increase in soot mass with the ambient temperature. However, computed steady-state mass values are underestimated for the 850 K condition while they are overestimated when ambient $T_{amb}$ is increased to 1100 K. Such trend is not completely consistent with the prediction of the LOL which is illustrated in Figure 9.

A possible reason for such discrepancy can be mainly related to the temperature dependency of the model constants describing the soot formation. Such observation is confirmed by the results illustrated in Figure 18, where the soot mass evolution is reported at 900 K ambient temperature for three different tested oxygen concentrations. Computed results are in rather good agreement with experimental data. In particular, the highest amount of soot was formed for the 15% ambient oxygen concentration: under such condition, the flame stabilizes at a relatively short distance from the nozzle and there is a reduced amount of O$_2$ available for soot oxidation. Similar amount of soot mass was found for the other two conditions. In the O$_2$ = 21% condition, an increase in oxygen concentration enhances the soot oxidation rate. Reduction of O$_2$ to 13% decreases the soot formation rate since the flame stabilizes at a higher distance from the nozzle compared to the other two conditions.

**Conclusion**

Two different Diesel combustion models which both use offline chemistry tabulation, namely the ADF and the FGM, were compared and assessed in terms of global heat release rate indicators and flame structure by simulating the ECN Spray A experiment in different conditions, including the variation of ambient temperature and oxygen concentration. The main difference in the theoretical assumptions beyond these models is in the way reaction rates are estimated during the table generation process: in ADF they are based on homogeneous auto-ignition calculations while in FGM unsteady counter-flow diffusion flames are solved. The latter is obviously much more demanding in terms of CPU time such that in the conventional model formulation a single strain rate is considered assuming that ID is not affected by it in a relatively large range of values. In the ADF tabulation, instead the stoichiometric scalar dissipation rate $x_{st}$ and the variance mixture fraction $Z^{\prime 2}$ are included to account for turbulence–chemistry interaction.

Models were tested considering n-dodecane sprays under constant-volume combustion conditions and considering variation of ambient temperature and oxygen concentration. It was observed how in general ignition occurs in rich region and then the reactions move toward stoichiometric zones. ADF results are clearly influenced by the turbulence–chemistry interaction: $x_{st}$, $Z^{\prime 2}$ and the reactivity play a fundamental role. The study of the main combustion tracers has given...
significant information about IDs, LOLs and flame structure. Agreement with experimental data was generally good for both models, apart for the prediction of the LOL at low temperature given by the ADF model, probably due to an excessive diffusion of the progress variable, and for the prediction of the ID under the same condition for the FGM approach. To improve this aspect, a novel FGM implementation, 5D-FGM, which also include strain rate effects, was proposed: ID was better estimated since chemical reactions occur in presence of low strain rates for such low reactivity condition.

Finally, a preliminary assessment of the soot distribution given by the ADF model was proposed: qualitative trends agreed with the observed data, but further investigations are required to improve the quantitative estimations of soot mass, especially when varying the ambient temperature.

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