Research Article

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Implementation of the Semi Empirical Kinetic Soot Model Within Chemistry Tabulation Framework for Efficient Emissions Predictions in Diesel Engines

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Abstract: Soot prediction for diesel engines is a very important aspect of internal combustion engine emissions research, especially nowadays with very strict emission norms. Computational Fluid Dynamics (CFD) is often used in this research and optimisation of CFD models in terms of a trade-off between accuracy and computational efficiency is essential. This is especially true in the industrial environment where good predictivity is necessary for engine optimisation, but computational power is limited. To investigate soot emissions for Diesel engines, in this work CFD is coupled with chemistry tabulation framework and semi-empirical soot model. The Flamelet Generated Manifold (FGM) combustion model precomputes chemistry using detailed calculations of the 0D homogeneous reactor and then stores the species mass fractions in the table, based on six look-up variables: pressure, temperature, mixture fraction, mixture fraction variance, progress variable and progress variable variance. Data is then retrieved during online CFD simulation, enabling fast execution times while keeping the accuracy of the direct chemistry calculation. In this work, the theory behind the model is discussed as well as implementation in commercial CFD code. Also, soot modelling in the framework of tabulated chemistry is investigated: mathematical model and implementation of the kinetic soot model on the tabulation side is described, and 0D simulation results are used for verification. Then, the model is validated using real-life engine geometry under different operating conditions, where better agreement with experimental measurements is achieved, compared to the standard implementation of the kinetic soot model on the CFD side.

Keywords: Computational Fluid Dynamics; Flamelet Generated Manifold; Diesel combustion; Soot modelling

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1 Introduction

Diesel combustion is still very important in the modern-day world, as it is being used in many fields, from transportation to energy production and heavy-duty applications. However, due to strict emission regulations, it is necessary to optimise it in terms of produced NOx and soot particles, which is often on the opposite sides of the spectrum: emission-reduction techniques tend to increase soot emission while reducing NOx emission, and vice versa [1].

CFD modelling has become an essential part of such efforts, and it can be especially useful in the engine design process. Typically, the number of parameters available for optimisation of the combustion is very large: injection strategies and ignition timings, Exhaust Gas Recirculation (EGR) amount and pressure, boost pressure, valve timings etc. To optimise all these parameters, an accurate and predictive combustion model is necessary, which includes flame front chemistry as well. However, due to the inherent complexity of diesel combustion which includes thousands of species and tens of thousands of reactions between them, computational power that is necessary quickly grows beyond practical limits, especially in the industrial environment. In addition, it is necessary to have predictive models for emissions, which is a very complex phenomenon as well. Because of that, it is very important to optimise combustion modelling in terms of CPU usage, while keeping the accuracy and predictivity.

The FGM combustion model [2] offers a good framework to achieve that: it allows including state-of-the-art

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reaction mechanisms in CFD simulations at very practical CPU cost. This is done by using chemistry tabulation, a pre-processing technique that consists of pre-computing the combustion chemistry, storing relevant data in a look-up table and interpolating from this table during the CFD simulation. In this work, the AVL FIRE™ CFD software is used to compare predictions of the FGM model [3] and the detailed chemistry model to experimental data from a light-duty Diesel engine.

In order to correctly and efficiently predict the soot formation during the combustion, an appropriate soot model is necessary. Soot modelling is a very large science field, as processes involved are complex and hard to describe. Although investigations of the soot emissions for gasoline engines exist [*e.g.* 4], in this work only soot modelling for diesel engines is considered. Soot models can be divided into three subcategories [5]: empirical models, semi-empirical models and detailed models. Empirical models are the simplest ones, presented by equations that are adjusted to match experimental soot profiles [6]. But, since they do not predict a time evolution of soot particles, but rather just a final value at exhaust for the engine, these models are of very limited use in CFD calculations and are used mainly for testing purposes. Opposite of the empirical models, detailed models are trying to capture as many details of the soot formation processes as possible. As such, these models can provide valuable insight into the physical and chemical processes but are often very expensive in terms of CPU resources. For example, Pang *et al.* showed a six-step phenomenological soot model with particle dynamics and PAH chemistry integrated into the model [7]. It covers particle inception, surface growth, coagulation and surface oxidation, as well as soot precursor formation and oxidation. It is an extensive model, but its usage is prohibited in industrial environments due to high computational complexity. Detailed model of Tao *et al.* [8] overcomes some of the high CPU usage problems, by reducing the chemistry: it is assumed that fuel has only one component. This means that only n-heptane kinetics are used for oxidation chemistry. In addition to that, a simplified chemical mechanism with 65 species and 273 elementary reactions is used. It starts with fuel pyrolysis and then acetylene is formed. Formation reactions of PAHs from acetylene are considered as the initial stage for soot formation, making acetylene the soot precursor in this model. The model was successfully applied to analyse the soot distribution structure in a conventional diesel for a benchmark heavy-duty diesel engine (Cummins). Vishwanathana and Reitz went in the same direction of reducing the complexity, by developing a model based only on four fundamental steps: soot inception through a four-ring PAH species, surface growth of acetylene, coagulation of acetylene to form soot, and soot oxidation via oxygen and OH [9–11].

Semi-empirical soot models are in between empirical and detailed model, regarding both soot formation details that are covered and computational complexity. The model devised by Hiroyasu *et al.* is one of the most widely used semi-empirical models [12]. Due to its relatively simple nature and connection with the CFD tools, combined with providing insight into the bulk distribution and transport of the soot in the high-temperature combustion environments of conventional diesel engines, this model is very popular within combustion community and therefore very important in the soot modelling analysis. However, since formation formula of Hiroyasu's model contains no dependence on the type, composition or structure of fuel, it has been proven that it is not suitable for diesel combustion soot predictions [13]. The recent model of Hiroyasu-Nagle and Strickland (HNS) [14] improved that and was successfully used for Diesel fuels.

In the present work, a semi-empirical soot model is used (the 'kinetic soot model'), which is then implemented on the tabulation side. This means that the model uses species input from the direct chemistry and soot mass fraction is then stored in the table in the same way as for any other chemical species. A look-up procedure is used to retrieve this value during the online CFD simulation.

2 Model description

Since it is necessary to model both combustion and soot emissions, two approaches are discussed here: FGM implemented in the tabulation framework (combustion model), and kinetic soot model implemented in both CFD and tabulation (in order to compare the two, the main contribution of this work is then finally tabulated kinetic soot model).

2.1 Combustion modelling approach

The applied combustion model has two main features:

- Chemistry tabulation based on auto-ignition trajectories of homogeneous fuel/air mixtures, computed with detailed chemical reaction mechanisms.
- Presumed-PDF Turbulence-Chemistry Interaction (TCI) modelling

The FGM look-up tables are built up with the software mentioned above, which is a dedicated tool for the generation of CFD look-up tables for advanced combustion mod-

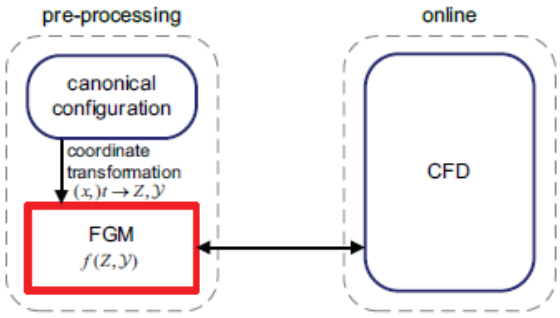

Figure 1: Scheme of FGM model, taken from [15]

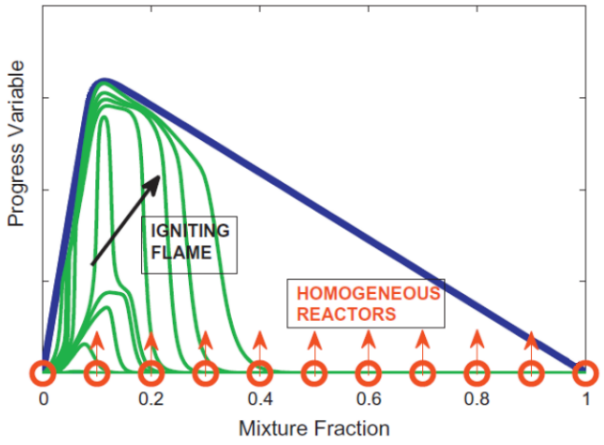

Figure 2: Homogeneous reactor calculations. Adapted from [3]

elling. The look-up tables have up to six dimensions: pressure, fresh gas temperature, mixture fraction (Z), mixture fraction variance, progress variable and progress variable variance.

For calculation of the chemistry at the tabulation side, 0D homogeneous reactor simulations are used, with these constraints:

- all variables are functions of time only
- the system is closed adiabatic and isobaric
- conservation of mass

The mean mixture fraction equation can be described as follows:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{Z}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{Z}\right)=\frac{\partial}{\partial x_i}\left(\overline{\rho}\left(D+D_T\right)\frac{\partial\tilde{Z}}{\partial x_i}\right)+\overline{\dot{\omega}}_{vap}$$

The main properties of the mixture fraction are, that it is zero in the oxidiser and unity in the fuel, that it is not consumed by chemical reactions, that it is equal to the fuel in the non-reacting case and that it has a spray source term for liquid fuels.

For considering the TCI the variance of the mixture fraction is calculated. It can be described by the following equation:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{Z^2}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\widetilde{Z^2}\right)=\frac{\partial}{\partial x_i}\left(\overline{\rho}\left(D+D_T\right)\frac{\partial\widetilde{Z^2}}{\partial x_i}\right)+2\overline{\rho}D_T\left(\frac{\partial\tilde{Z}}{\partial x_i}\right)^2-\overline{\rho}\tilde{\chi}_Z$$

The scalar dissipation rate $\tilde{\chi}_Z$, which is derived from the above variance, is:

$$\tilde{\chi}_Z=2\frac{\varepsilon}{k}\widetilde{Z^2}$$

For the progress variable, which describes how far chemical reactions have proceeded, several formulations are possible. *E.g.* it is often defined as a linear combination of species like shown here:

$$Y_C=\frac{Y_{CO}}{W_{CO}}+\frac{Y_{CO2}}{W_{CO2}}$$

where major species CO and CO_2 are used, weighted by their respective molecular weights. In the applied approach, an automated procedure can be used to define the progress variable. The normalised progress variable can then be written as:

$$c=\frac{Y_C}{Y_C^{EQ}}$$

Transport equations for the normalised mean progress variable and its variance are formulated in a similar way as shown for the mixture fraction above:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{c}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{c}\right)=\frac{\partial}{\partial x_i}\left(\overline{\rho}\left(D+D_T\right)\frac{\partial\tilde{c}}{\partial x_i}\right)+\overline{\rho}\overline{\dot{\omega}}_c$$

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{c''^2}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\widetilde{c''^2}\right)=\frac{\partial}{\partial x_i}\left(\overline{\rho}\left(D+D_T\right)\frac{\partial\widetilde{c''^2}}{\partial x_i}\right)+2\overline{\rho}D_T\left(\frac{\partial\widetilde{c''^2}}{\partial x_i}\right)^2-\overline{\rho}\tilde{\chi}_c$$

$$\tilde{\chi}_c=2\frac{\varepsilon}{k}\widetilde{c''^2}$$

2.2 Soot emissions modelling

The soot emissions have been calculated by a kinetic soot model [16], which refers to reduced soot chemistry for the formation and oxidation processes. The reduced chemistry has been derived from a detailed chemical model for soot formation and oxidation. Detailed model [17] can produce soot yield curves from 0D calculations, giving soot concentration over multiple temperature points for a given pressure and equivalence ratio. Kinetic soot model is represented by three reactions:

- reaction of soot formation:
  $C_{cn}H_{hm} + C_{cn}H_{hm} = 2(cn)C + \text{Product (I)}$
- reaction of soot oxidation by oxygen:
  $C + C + O_2 = \text{Product (II)}$
- reaction of soot oxidation by water
  $C + H_2O = \text{Product(III)}$

where soot is represented by the C atom and product is attributed to either CO_2 or N_2 in order to keep minimal the number of reactive species. Each reaction is characterized by the reaction rate W_i (i = I, II, III):

$$W_i = A_i exp\left(\frac{E_i}{RT}\right)\prod[X_i]$$

where T is the temperature, E_i is the activation energy, and $\prod[X_i]$ are the products of volume fractions of species participating in the reaction. The rates of reactions (I), (II), and (III) are written in the form:

$$W_I = 2\,(cn)\,K_I\left[X_{C_{cn}H_{hm}}\right]\left[X_{C_{cn}H_{hm}}\right]$$

$$W_{II} = 2K_{II}\,[X_C]\,[X_C]\left[X_{O_2}\right]$$

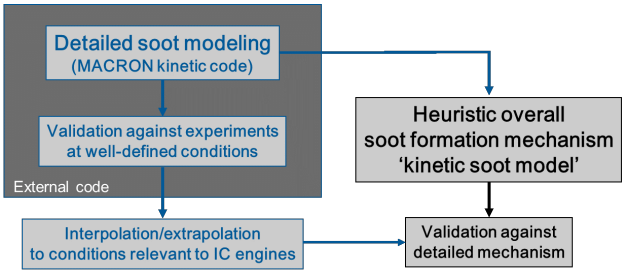

Figure 3: Flow chart of the kinetic soot model

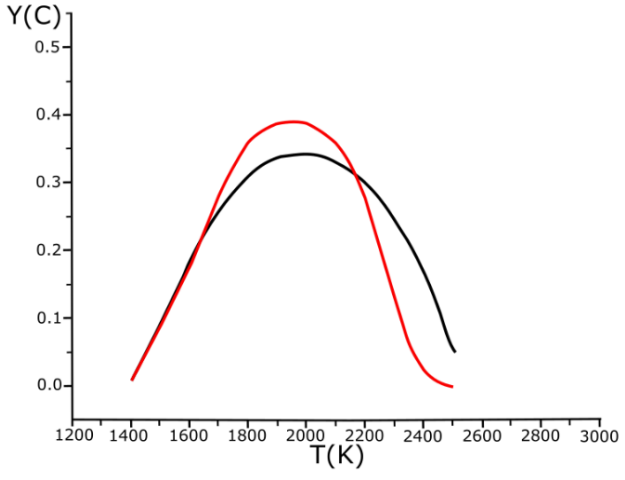

Figure 4: Example of a soot yield curve (black) from detailed model and fitted curve (red), for 10bar pressure and equivalence ratio of 2 at time t=3ms

$$W_{III} = K_{III}\,[X_C]\left[X_{H_2O}\right]$$

where $K_i = A_i \exp\left(-E_i/RT\right)$. Kinetic parameters A and E for reactions (I), (II) and (III) are optimized for different fuels, pressures and temperatures in order to fit the detailed model soot yield curves (Figure 4). Fuel, O_2 and H_2O species concentration calculated by CFD code are used as an input to the model in order to calculate the reaction rates of (I), (II) and (III).

In FGM approach however, the input for this model is a 'virtual fuel' species which is representative of not only the fuel species itself but all relevant fuel-related radical species.

This model has been implemented on the tabulation side: based on the standard input to the model (virtual fuel for soot formation and O2 and H2O for soot oxidation), soot concentration is calculated during the chemistry calculation (*i.e.* within Perfectly Stirred Reactor (PSR) 0D solver) and stored in the table in the same manner as other chemistry species. Retrieving is done during the online CFD calculation (again, same as for chemistry species).

3 Model verification

Before running a validation using a real-life test case, a basic verification of the model implementation has been done using simple theoretical setups. Purpose of these setups is to test basic behaviour and to have a starting point in testing. Results are then checked against (theoretically) expected results. Each test case is run with n-Heptane as a fuel, and JIA mechanism (reduced n-Heptane, 45 species) used for chemistry [19].

3.1 Combustion verification

For combustion verification, four different setups are used, with increased complexity and details added for testing: 0D box, stratified box, GasJet and SprayH. Each setup is discussed in the following subsections.

3.1.1 Homogeneous box

This 0D setup is very simple and equal to homogenous reactor already described in paragraph 2, so it has to yield the same results (given the same initial conditions). Furthermore, adiabatic flame temperature (which is well known for this simple setup) should be reached (within expected error margin). The numeric setup itself consists of

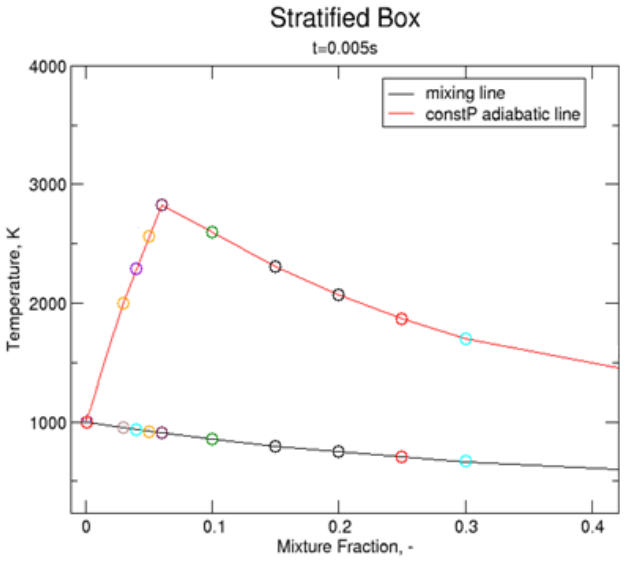

Figure 5: 0D results

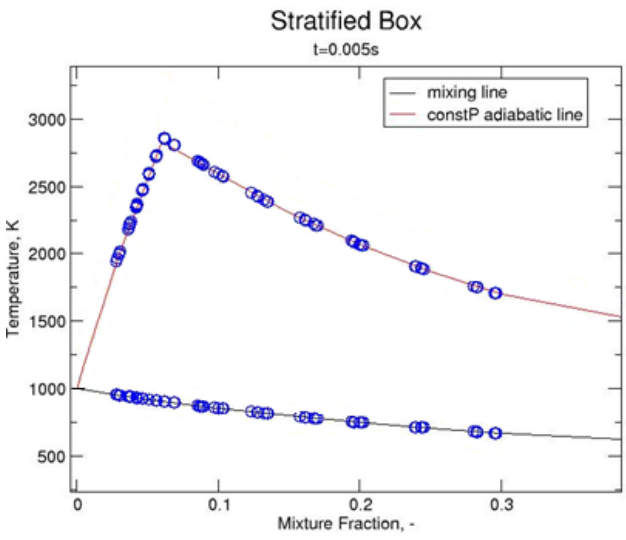

Figure 6: Stratified box results

a box (of arbitrary metric and mesh size, in our case is 1 cm inside length and 64 cells) initialized with initial pressure, temperature, fuel mass fraction (*i.e.* mixture fraction), oxidizer concentration and progress variable set to 0, since we are starting with unburnt mixture. Fuel used is n-Heptane, and the mechanism is a simple one-step reaction. Simulation runs for 5 ms (although equilibrium temperature is reached long before that). Results are then plotted onto Z-T graph, with plotted theoretical limits – mixing and adiabatic line (*i.e.* fresh gas and adiabatic temperatures for a given Z range). Constant pressure (open boundaries) setup is used with 10 points in (P, T, Z) space, each initialised from a mixing line for a given fuel. Results for both setups are presented in Figure 5, showing the exact match with expected values.

3.1.2 Stratified box

After basic combustion test was performed using the 0D setup, the next step is to check how is mixing influencing combustion. This is done by using stratified box setup: same 10 initial points used for the homogeneous box but used at the same time – each point occupies one part of the box (Figure A1). Results are expected to be within given limits – equilibrium temperature points should be on the adiabatic temperature line (Figure 6).

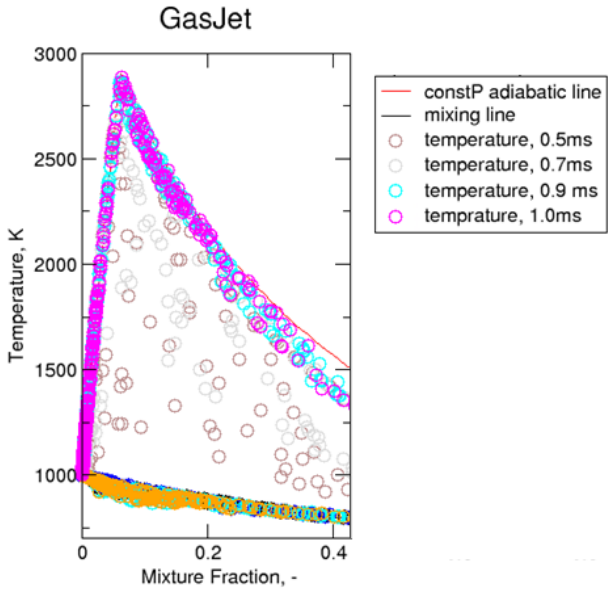

Figure 7: GasJet results

3.1.3 Gas jet

Purpose of this setup is to test fuel injection, but with the setup that is simpler than typical spray setup: fuel is entering the box at high speed, through a narrow hole. Initial and boundary conditions setup is presented in Figure A2. Then the evolution and the final temperature are plotted onto the Z-T graph (Figure 7). Results are within expected limits.

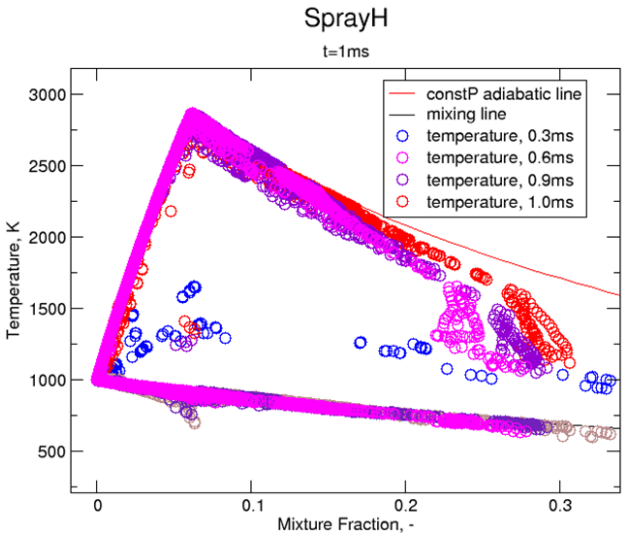

Figure 8: SprayH setup results

3.1.4 SprayH

This setup is used to test basic spray configuration (configuration can be found at [20], ECN database). Results are presented in Figure 8 and expected Z-T profile is matched for a condition present in realistic engine setup. For very rich conditions (mixture fraction >0.3, unrealistic for the engine conditions), this setup needs more time to converge completely to the adiabatic temperature line for each point. Final time used here was 1ms, which is enough for engine conditions which will be tested later. Also, a few points are below mixing line, which is attributed to the numerical inaccuracy of the setup (*i.e.* box setup that is used should be more refined in term of the cell size), but it is still sufficient for basic verification: given the total number of points plotted here for the converged state, points below mixing line present less than 0.1%.

3.2 Soot model verification

After basic combustion has been checked and validated against idealised, theoretical cases, the same was done for implementation of the soot model on the tabulation side. For this purpose, same 0D setup was used, but in three configurations (in each configuration, the soot model is directly coupled with 0D homogeneous reactor solver on the tabulation side):

(1) soot mass fraction plotted as an output from the kinetic model
(2) same as previous, but soot mass fraction is firstly tabulated, and then retrieved from the table (using standard tabulation verification tool, *i.e.* without running CFD)
(3) both previous steps were done, but now soot is fetched during CFD calculation – this represents real case usage scenario

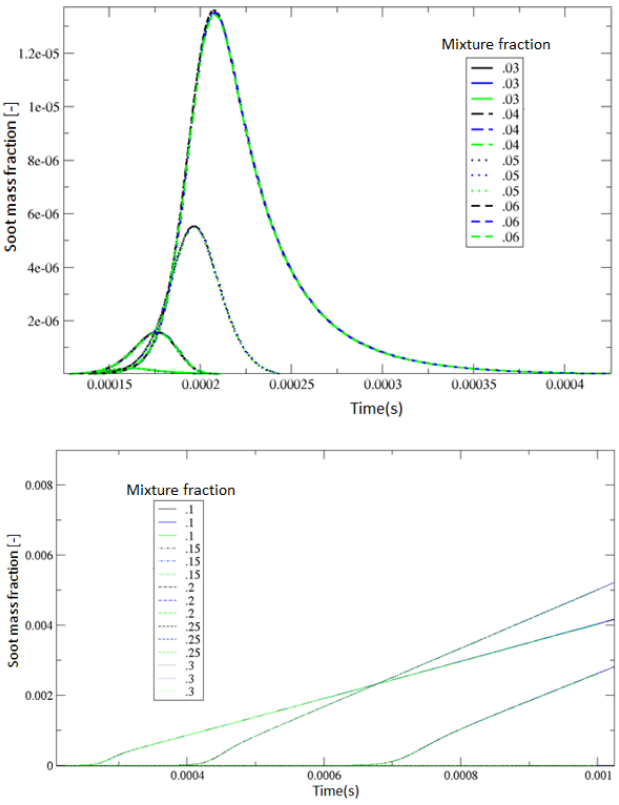

Figure 9: 0D setup results for soot mass fraction, fuel lean and rich conditions

This workflow ensures that the implementation is properly validated for each critical part of the model. All three outputs should give the same result. Tests were done for six different equivalence points, three for lean conditions and three for rich conditions. Results are shown in Figure 9, where case (1) is presented with black lines, case (2) with blue lines, and case (3) with green lines. All cases are showing a perfect match, confirming the validity of the model implementation. Also, lean cases are fully oxidized for the time scale relevant in engines, while rich cases are showing constant soot production. For that reason, rich cases were run for longer times (up to 1 ms), long enough to catch realistic time scales in the engine conditions. Therefore, the presented results show expected trends for relevant engine cases.

Table 1: Engine characteristics

Bore, mm	81
Stroke, mm	93,15
Conrod, mm	147
Compression ratio, -	16,5
Injection system / injector	Bosch CR / 7 holes, 145 deg

4 Engine simulation and validation

The validation of the model has been performed using a standard passenger car size diesel engine under real-life conditions. This engine is equipped with a modern common rail injection system and for it exists a large database of measurements done by AVL, spanning different load points, injection strategies, EGR levels etc.

4.1 Engine and calculation setup

The engine characteristics are provided in Table 1. All initial and boundary conditions have been closely checked in order to be consistent for the purpose of CFD validation.

In this work, different load scenarios were considered. Data for the given cases are summarized in Table 2. All cases have 4 injections, shown in Figure 10: 2 pilot injection, 1 main and 1 post-injection, with injected fuel mass percentages shown in Table 3. Figure 11 shows the computational mesh, which has been generated automatically based on the contour of the piston bowl. Due to the centrally mounted injector, rotational symmetry can be assumed. Therefore, just a segment of the geometry, which contains one injection hole, has been modelled. The resulting mesh size varies between 80.000 and 150.000 cells. Turbulence is modelled using the k-zeta-f model with hybrid wall treatment for turbulence and standard wall function for heat transfer. The temperature boundary section is set to a constant value. The spray is modelled using an Eulerian-Lagrangian approach with the Dukowicz evaporation model and the Wave spray breakup model (C1=0.61, C2=18, C3=1, C4=0.1, C5=0.3). Drag is modelled using Schiller Naumann, turbulent dispersion is enabled and particle interaction is not considered. More details about the applied models can be found in [18].

Table 2: Load points used for validation

Case	Speed(RPM)	IMEP(bar)	EGR
3000_6	3000	6	17%
2000_6	2000	6	33%
2000_2	2000	2	43%
1000_4	1000	4	40%

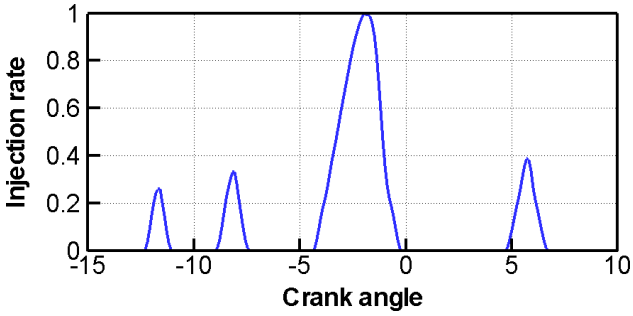

Figure 10: Injection timing

Table 3: Injected fuel mass

Injection #	Injected mass distribution [%]
1	5%
2	9%
3	74%
4	13%

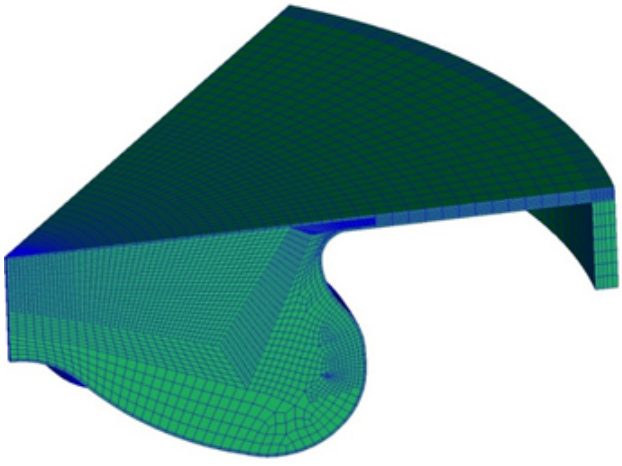

Figure 11: Computational (sector) mesh

4.2 Investigation of chemistry mechanisms

As previously stated, during the tabulation a chemistry mechanism is used for calculation of the chemistry for the 0D homogeneous reactor. Of course, given the fuel species, any verified mechanism can be used, and presented here is a study of different mechanisms used for FGM model and

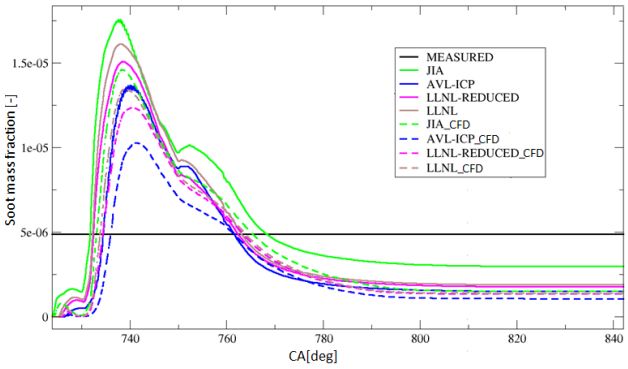

Figure 12: Comparison of soot mass fraction for the different mechanism used

Figure 13: Comparison of the measured data with FGM model with embedded soot model for different load scenarios

subsequently soot model (which uses input from the chemistry in terms of fuel species and oxidiser concentrations). Additionally, a set of calculation was performed where kinetic soot model was implemented in the CFD code (in contrast to being on tabulation side). This enables a comparison between the performance of two different implementations as well.

Mechanisms used are:

- JIA mechanism [19]
- AVL proprietarily mechanism [21]
- Lawrence Livermore National Labs mechanism, full and reduced [22]

The case used for calculations is 1000_4, and soot mass fraction is used for comparison (plotted as a function of crank angle degree during the combustion and exhaust phase). Results are presented in Figure 12. Black line represents measured value at the exhaust valve open event. Since measurements provide only final (single) value at the end of a combustion event, a comparison is made in terms of how close the final calculated values are matching that value. Tabulation side soot values (full lines) are in all cases (slightly) better than CFD ones (dashed lines), with JIA mechanism giving the best overall results. Further investigation is necessary in order to check why other mechanisms are not performing as well, but this is a clear confirmation that the tabulation side calculation of the soot performs better than when implemented directly in the CFD. This can be attributed to better input to the kinetic soot model itself: fuel and oxidiser species concentrations are used directly, instead of using CFD ones, where a certain error is introduced due to the tabulation process. Also, given that the JIA mechanism is performing the best in term of soot predictions, it is used for calculation of different load points presented in the next subsection.

4.3 Emission result analysis

For comparison with the measured data, peak pressure, the crank angle where 50% of the fuel charge is burnt (CA50) and soot in terms of the smoke number are used. Then, different load cases were tested in order to check combustion and soot values for different in-engine conditions (corresponding to the basic tests performed, which were ranging for very lean to very rich). Also, each case has a certain level of EGR, as shown in Table 2. Results are presented in Figure 13.

Firstly, the main combustion quantities are checked: peak pressure is captured very well, with very small error compared to the measured value. Also, CA50 is giving

Table 4: Comparison of calculation times between FGM and direct approach

Mechanism (Species / Reactions)	Calculation Time / FGM	Calculation Time / direct chemistry calculation
JIA(45 / 177)	3.3 h	4.5 h
AVL (160 / 1540)	4.0 h	25 h
LLNL(658 / 2827)	6.2 h	12.1 days

a good agreement, which means that combustion is well predicted with the FGM approach. Finally, soot is checked against measured data in terms of smoke number (FSN); calculated values are in good agreement with the measured data.

One of the big advantages of using tabulated chemistry compared to direct approaches is the computational time needed for the calculation. Average CPU time per case, with tabulation included, was around three hours. At the same time, FGM keeps the accuracy of the direct approach. Given that typical value for direct approach (using the same CFD software and same hardware) for a Diesel sector is around one day (and depending on the mechanism used, it can be weeks), it is clear, that FGM has a big advantage, especially in industrial environment. Table 4 summarises calculation times for three mechanisms used (AVL and LLNL are reduced in this analysis).

5 Conclusion

Tabulation framework coupled with the kinetic soot model was presented. Using an FGM model, combustion and soot emissions for Diesel fuel were simulated and then verified against basic academic cases. n-Heptane was used as a surrogate fuel. Theoretical values were successfully reproduced, after which real-life use cases were tested. Applying the setup from a standard Diesel passenger car engine, first a study of different chemistry mechanisms used for 0D calculations during tabulation, was performed. For comparison with the measurements, the final value of the soot mass fraction at the exhaust valve open event was used. It showed that for five different mechanisms, tabulation side soot model was giving better predictions than the CFD side soot model. The same investigation showed that the tabulation with JIA mechanism is giving the best predictions. Therefore, this mechanism was used for further tests on four different load cases of the same engine.

Four different load points were tested, and pressure, CA50 and soot in terms of the smoke number were used as validation quantities. First two showed very good match with experimental data, proving that FGM can capture combustion in Diesel engines accurately and efficiently. Then, soot was compared with measurements using the smoke number, and it provided a very good match.

Finally, an overview of the calculation times was given, showing a very big advantage in terms of CPU resources when using FGM, especially in the industrial environment.

Overall, FGM coupled with kinetic soot model is providing a very good framework for investigations of Diesel combustion and can be used effectively for design frontloading in the industry. Since AVL databases provide a large number of measured cases, the next step in this investigation is to test the presented model on more cases to check its predictivity on a larger scale.

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A Appendix

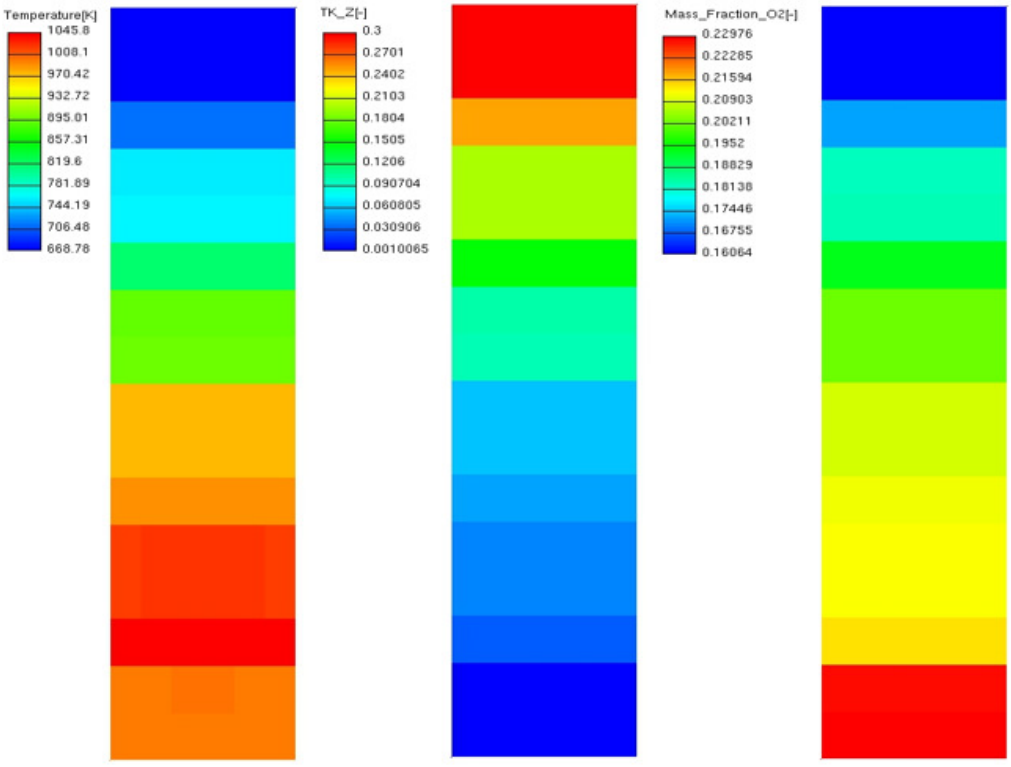

Figure A1: Stratified box setup

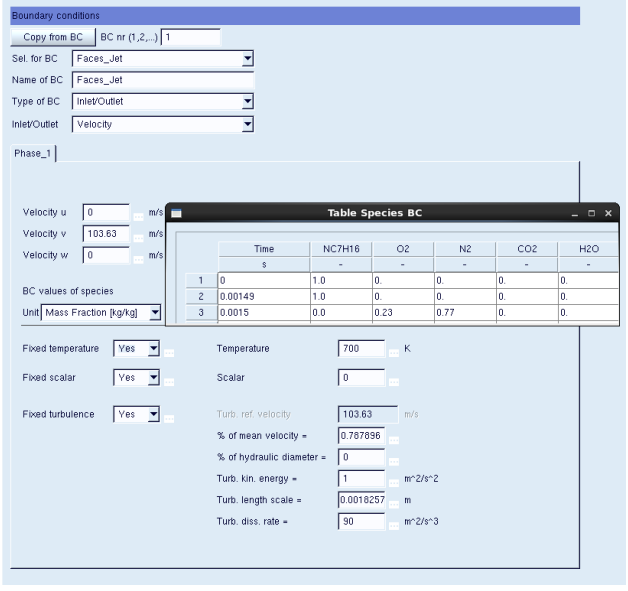

Figure A2: GasJet setup