

Simplified and Detailed Chemistry Modeling of Constant-Volume Diesel Combustion Experiments

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ABSTRACT

The high complexity of the interplaying physical and chemical phenomena occurring in Diesel combustion has brought an increasing interest versus experimental and computational fundamental studies. A relevant contribution to the availability of suitable and accessible experimental data is represented by the Engine Combustion Network database, which are of great interest for model development and validation because of the well-defined boundary conditions and the wide range of conditions employed [1].

In this paper the authors implemented into a unique open-source CFD code two different combustion models of different complexity and applied them to simulate a selection of significant test cases from this database. The first one is an extension of the Eddy Dissipation Model and it can be used as a development tool because of its limited computational demand. The second one is the Perfectly Stirred Reactor model and directly employs detailed chemical kinetics in each computational cell, making use of the ISAT tabulation to reduce the computational time. Global heat release rate, flame lift-off lengths and flame structure (HCHO, PAH and soot distributions) are compared with the available experimental data.

INTRODUCTION

Diesel combustion modeling is a very challenging task due to the complex interplay of turbulence and chemistry which determine auto-ignition, flame structure, fuel oxidation, local quenching and pollutant formation. Despite the fact that each of these aspects has been matter of investigation for decades, a deeper understanding of many fundamental phenomena is still needed together with the achievement of time efficient

CFD tools which can support the design of the next generation Diesel and HCCI engines. For these purposes, a fundamental requirement is to implement the existing different models into the same CFD code and apply them to the identical conditions [2, 3]. In this contest, a relevant contribution to the availability of suitable and accessible experimental data is represented by the Engine Combustion Network database. It consists of series of constant-volume diesel combustion experiments, including a wide range of ambient environments which span those typically experienced in a diesel engine [1].

On the basis of these considerations, the authors intend to contribute to develop a CFD platform to be used for fundamental studies to compare results of different models when applied to simulate public domain experiments. To these ends, the authors have contributed over the last years to the development and application of the multipurpose CFD code OpenFOAM [4, 5], which additionally has the advantage to be fully open-source and written in an highly efficient object-oriented programming allowing an easy implementation and testing of new models. In this paper, two different combustion models were implemented and validated. The first is a modified version of the Eddy Dissipation Model, coupled with an ignition treatment to evaluate the ignition delay. Interest in such a simplified approach arises because of its suitability for industrial application, due to the reduced computational cost. The introduction of ignition delays tabulated from complex chemistry is discussed to overcome known limits of this model, without relaxing the fast chemistry assumption for the rest of the combustion. As alternative, a Perfectly Stirred Reactor model has been implemented, assuming homogeneous mixture within each computational cell in which detailed chemical kinetics is directly employed. This approach implicitly suggests kinetics controlled combustion in each cell. It becomes thus of great interest to analyze the

results of this model when applied to simulate the auto-ignition and following non-premixed turbulent combustion, varying significantly the environment conditions. In fact the good or bad agreement achieved with the experimental data might help the understanding of the occurring combustion regimes and possible existing turbulence/chemistry interaction. Additionally, the employment of a complex chemistry approach allows to investigate the cool flame near the lift-off length by comparing the formaldehyde and OH distributions with recent experimental findings [6]. Semi-empirical soot models have finally been implemented so that it was possible to exploit the influence of the lift-off height predictions of the downstream soot production.

COMPUTATIONAL MODEL

Discretization accuracy, solver efficiency, geometry-handling capabilities and computer implementation are paramount numerical requirements which have to be taken into account by the numerical analyst to assemble efficient algorithms [7]. In the previous section, the authors have already mentioned their use and development of the OpenFOAM code for the proposed fundamental studies. In fact its object-oriented structure allows the code designer to create a more manageable software, with lower maintenance cost, extensive code re-use, fewer bugs and easier extendibility. The high complexity of the physical and chemical models and the existing interrelations make the numerical solution methodology play a role of equal importance as the mathematical modeling. It results that the main features of the programming language (i.e. C++ for OpenFOAM) assume great relevance. OpenFOAM makes an extensive use of *data abstraction*, *object orientation* and *operator overloading*. They respectively allow the designers to introduce new data types appropriate for the problem (i.e. mesh, spray, chemistry solver, geometric fields,...), bundling of data and operations into classes, protecting the data from accidental corruption and creating class hierarchies and finally the operator overloading provides a natural syntax for newly defined classes and generic programming. More details about the structure of the OpenFOAM code can be found in [4, 5, 8].

Focusing on the Diesel modeling, OpenFOAM has been recently used for Lagrangian spray modeling. The code already includes most of the widely used sub-models for spray breakup, fuel injection, droplet collisions, evaporation and turbulent dispersion. In this work, a constant spray angle is used in the simulations, while the initial droplet diameter was derived by the injector diameter and its area contraction coefficient [9]. Both the Kelvin-Helmoltz and Rayleigh-Taylor mechanisms are accounted for to model the spray breakup [10]. The Ranz-Marshall correlation [11] is used to model the droplet evaporation. Droplet to droplet interactions and turbulence dispersion effects are neglected. Further details about the spray implementation and validation can be found in [9, 12, 13, 14, 15].

In this work two different combustion models were implemented into the code and discussed. The first one is an extension of the Eddy Dissipation Model and it can be used as a development tool because of its limited computational demand. The second one is the Perfectly Stirred Reactor model [16] and directly employs detailed chemical kinetics in each computational cell. For both approaches, the RNG $k - \varepsilon$ is used to model turbulence [3, 9].

MODIFIED EDDY DISSIPATION MODEL (EDM+ID)

In Diesel combustion, the fuel is injected into hot, compressed air and auto-ignition plays an important role in the combustion and flame stabilization processes. After ignition, combustion is generally mixing-controlled [17]. For these reasons, the fuel reaction rate can be expressed as:

$$\bar{\omega}_F = (1 - \alpha)\bar{\omega}_{F,HT} + \alpha\bar{\omega}_{F,mix} \quad (1)$$

where α is used to switch from the auto-ignition ($\alpha = 0$) to the mixing-controlled combustion mode ($\alpha = 1$). Expressions of the two terms $\bar{\omega}_{F,HT}$ and $\bar{\omega}_{F,mix}$ are thus required.

A well known and simple way to account for high temperature auto-ignition in Diesel engines is to perform a time-integration of a fictitious intermediate specie $\tilde{Y}_{HI}$ which is transported through convection and diffusion. The growth rate of the progress variable $\tilde{Y}_{HI}$ is proportional to the amount of the fuel tracer $\tilde{Y}_{T,fu}$ in the mixed zone and is a function of the local self-ignition delay τ_{HT} , which depends on the fresh gas thermodynamic conditions. This value is typically estimated from an Arrhenius correlation [18], but this dependency is rather simplified and provides correct estimations of the ignition delay only in a limited range of temperatures, pressures and equivalence ratios. To overcome these limits, the approach of Pires De La Cruz [19] has been implemented in the code, computing ignition delay by a linear interpolation in a tabulated database whose values are the result of complex chemistry calculations, performed by the authors, with an extensively validated detailed kinetic scheme for n-heptane [20]. Details about the ignition delay database creation and validation are reported in the Appendix.

The fuel tracer represents the amount of fresh mixed fuel which would exist in the computational cell in absence of chemical reactions. It is a passive scalar because, by definition, it is neither consumed nor created by chemical reactions. The expression of $\bar{\omega}_{HI}$ is:

$$\bar{\omega}_I = \bar{\rho} \tilde{Y}_{T,Fu} \frac{1}{\tau_{HT}} \quad (2)$$

Ignition delay is reached when $\tilde{Y}_{HI} \geq \tilde{Y}_{T,Fu}$ and the expression for $\bar{\omega}_{F,HT}$ is:

$$\bar{\omega}_{F,HT} = Y_F / \Delta$$

The mixing-controlled fuel burning rate $\bar{\omega}_{F,mix}$ depends on the fuel ($\tilde{Y}_F$), oxidizer ($\tilde{Y}_O$), product mean mass fractions ($\tilde{Y}_P$) and on the turbulent mixing time, estimated from integral length scales as $\tau_t = k/\varepsilon$:

$$\bar{\omega}_{F,mix} = C_{mag} \bar{\rho} \frac{\varepsilon}{k} \min \left(\tilde{Y}_F, \frac{\tilde{Y}_O}{s}, \beta \frac{\tilde{Y}_P}{(1+s)} \right) \quad (4)$$

where C_{mag} and β are two model constants. In Equation 4, the reaction rate is limited by the deficient mean specie. When β is finite, this deficient specie may be combustion products to take into account the existence of burnt gases, providing the energy required to ignite fresh reactants. In the present work C_{mag} is set to 4, while β is 1, following [17]. When the Eddy Dissipation Model is coupled with an ignition treatment it is possible to predict both ignition and flame stabilization since fuel and oxidizer do not immediately ignite as soon as they meet [17].

The Eddy Dissipation Model implementation in OpenFOAM was validated by using the SANDIA bluff body flame test case [21, 22]. The experimental setup consists in a burner with a 3.6 mm methane jet and an outer diameter of 50 mm. The burner geometry was reproduced by using a 2D wedge of 22000 cells, refined close to its axis where the fuel is injected. The computational grid is shown in Figure 1(a). Figure 1(b) displays the temperature field: high temperature zones are found where the mixture is stoichiometric and this is in agreement with fundamental observation on jet flames [17]. Figures 2(a)-(b) show the radial distribution of the temperature for two different distances from the injector. The computed results agree with experiments in terms of maximum temperature locations, thus providing a correct description of the flame.

Once the models for ignition delay tabulation and mixing controlled combustion have been separately validated, it is possible to use the proposed combustion model to simulate a Diesel combustion process.

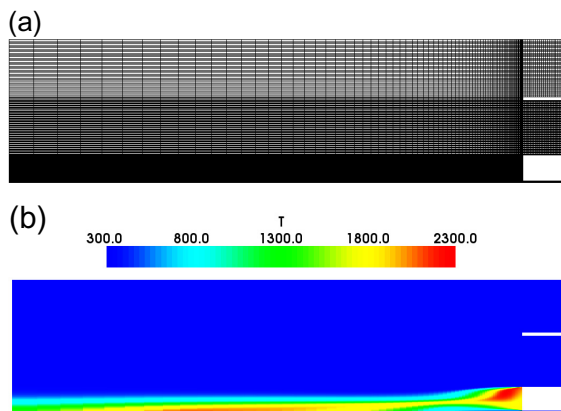


Figure 1: (a) Computational 2D mesh to simulate the SANDIA Bluff-Body Flame; (b) Computed temperature field.

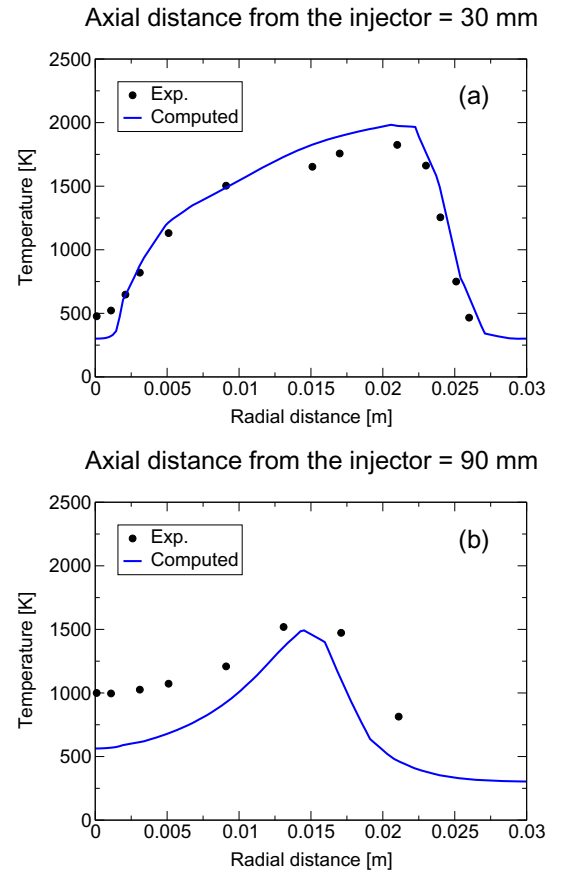


Figure 2: Computed and experimental radial temperature distribution at 30 mm distance from the fuel injector (a) and 90 mm distance from the fuel injector (b).

PERFECTLY STIRRED REACTOR MODEL (PSR)

In this model the mixture is assumed to be homogeneous within each computational cell, hence any sub-grid scale turbulence-chemistry interaction is neglected. This model has recently been applied in [2, 3, 23] for both combustion bomb and diesel engine simulations. The reactive mixture in each computational cell is treated as a closed system. When the chemical time scale is much lower than the fluid-dynamic time-scale, an operator-splitting [17, 24] technique is used: at the beginning of the each computational time an ODE stiff solver takes the thermodynamic conditions (T , p , Y_i) in each cell and integrates the chemical problem within the time-step, solving the specie and the energy equations. Then it updates the species mass fractions as:

$$Y_i^*(t + \Delta t) = Y_i(t) + \int_t^{t+\Delta t} \frac{\dot{\omega}_i W_i}{\rho} dt' \quad (5)$$

where ρ is the density, $\dot{\omega}_i$ is the reaction rate and W_i is the molecular weight of the species i . $Y_i^*(t + \Delta t)$ is the mass fraction of a chemical species calculated by the chemistry solver in each cell. In this work a multi-step, Semi-Implicit Bulirsch-Stoer solver, *SIBS*, was adopted [25]. Finally, the reaction rate $\dot{Y}_i$ is estimated as:

$$\dot{Y}_i = \frac{Y_i^*(t + \Delta t) - Y_i(t)}{\Delta t} \quad (6)$$

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The chemical mechanism can be provided to the OpenFOAM code in the CHEMKIN format [26], then suitable functions and libraries compute the reaction rates.

A skeletal mechanism with 32 species and 70 reactions was used to simulate the n-heptane chemistry. The kinetic scheme fully includes the mechanism by Patel et al. [27], but also incorporates 12 additional reactions to model the chemistry of acetylene (C_2H_2) and the formation of nitric oxides. The reactions for the C_2H_2 formation/destruction were taken from the complex kinetic mechanism by Golovichev et al. [20], while the thermal mechanism was used to model the chemistry of NO [28]. The original skeletal mechanism retains the main features of detailed mechanisms and has been extensively validated using constant-volume ignition delay data and engine combustion experiments [27].

The operator-splitting technique increases significantly the computational time, making use of detailed chemistry. For this reason, several approaches based on reaction rate tabulation were proposed in the past to reduce the computational time [19, 29]. The exploration of chemical look-up tables may become prohibitive because of memory access and multilinear interpolations. On the other hand, only a very small part of the table covers the accessed composition space. To overcome these difficulties, Pope and Young [30, 31] proposed to build the chemical table as needed on-the-fly during the computation (*in situ*). Further details about this numerical technique, named *ISAT*, in-situ adaptive tabulation, and how this algorithm was implemented by the authors into the OpenFOAM code are given in the Appendix.

The phenomenological soot model proposed by Moss [32] was implemented and applied in the simulations. It is based on a simplified representation of the processes of nucleation, heterogeneous surface growth, coagulation and oxidation as they apply to the balance between transport and production of the soot volume fraction f_v and particle number density n . The respective source terms are:

$$\frac{d}{dt}(\rho_s f_v) = \gamma n + \delta - \left(\frac{36\pi}{\rho_s}\right)^{1/3} n^{1/3} (\rho_s f_v)^{2/3} R_{tot} \quad (7)$$

$$\frac{d}{dt}(n/N_0) = \alpha - \beta (N/n_0)^2 \quad (8)$$

where α and β are the nucleation and the coagulation rates, while γ and δ represent respectively the impact of the surface growth and the nucleation on the soot volume fraction. Acetylene (C_2H_2) was used as the inception specie. The reader is referred to [2, 32] for further details about the expressions for the reaction rates.

EXPERIMENTAL VALIDATION

Experiments conducted in the SANDIA combustion chamber were used to evaluate the proposed models. It is an optically accessible, cubical vessel where spray-

combustion experiments are performed under ambient similar conditions to those occurring in a diesel engine at the time of injection. The fuel is injected by a common-rail injector mounted on one side of the chamber with a Mexican-hat injection profile. Sapphire windows provide optical access. A piezoelectric pressure transducer measures the vessel pressure during the experiments. The experimental apparatus is accurately described in [33, 34].

Firstly a mesh size investigation was performed in order to test the adopted spray models. Computed equivalence ratio distributions were compared with experimental optical images as function of time. Hence, a wide range of operating conditions was simulated, as summarized in Table 1. N-heptane was used as fuel and the injected mass for each case was taken from [1]. A comprehensive validation of the proposed models in terms of:

- heat release rate;
- flame lift-off location;
- flame structure;

is performed.

	ρ_{amb} [kg/m ³]	T [K]	[O ₂]
Case 1	14.8	1000	21%
Case 2	14.8	1000	15%
Case 3	14.8	1000	10%
Case 4	14.8	1300	21%
Case 5	14.8	900	21%
Case 6	14.8	750	21%

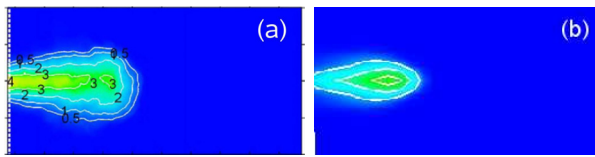
Table 1: Operating conditions simulated: initial ambient temperatures, densities and oxygen concentrations.

CASE SETUP

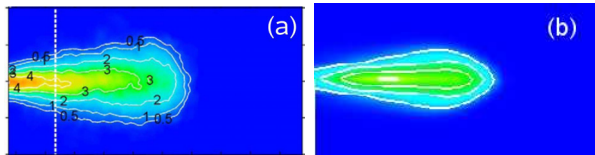
The computed fuel-air mixture distribution at the ignition time strongly affects the prediction of the combustion process: this is mainly due to known grid dependency of the spray models. Considering the axial-symmetric geometry, only a quarter of the combustion chamber was modeled. A mesh size investigation was performed and experimental optical measurements were compared with computed data for three different mesh sizes in the spray region: 2 mm, 1 mm, 0.5 mm. The 1 mm mesh provided the best results both in terms of vapor penetration and spray shape. Figure 3 compares the computed equivalence ratio distribution with the optical Rayleigh scattering images from [35] at the experimental auto-ignition time. Both the vapor penetration and the equivalence ratio distribution are captured rather well. Discrepancies can be found only in the very rich region where generally no ignition occurs, hence the prediction of the combustion process should not be influenced by this error.

The computational mesh adopted for the calculations is finally displayed in Figure 4. Three different cell sizes are

Case 1 : $O_2 = 21\%$, 0.42 ms ASI



Case 2 : $O_2 = 15\%$, 0.61 ms ASI



Case 3 : $O_2 = 10\%$, 0.106 ms ASI

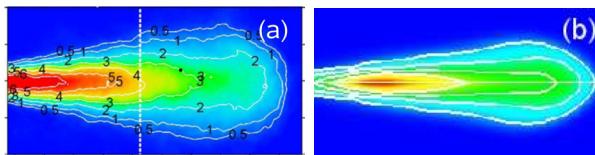


Figure 3: Comparison between experimental (a) and computed (b) equivalence ratio distributions for the cases 1-3. Experimental images reproduced with permission from [35]. Equivalence ratio range from 0 to 6.

used: 1 mm close to the spray axis, 4 mm close to the walls and 2 mm in the middle. In this way the mesh is very fine where combustion takes place and a coarse grid is used elsewhere, reducing the required computational time. The total number of cells is ~ 90000 . A time step of 1 microsecond has been used to better describe the spray evolution at the beginning of the injection phase.

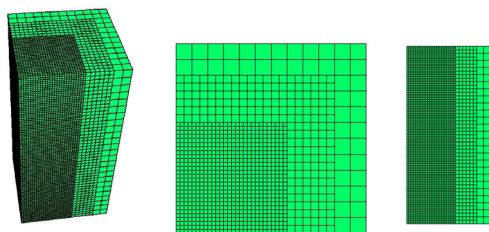


Figure 4: Computational mesh representing the SANDIA combustion vessel [1].

Finally, the ISAT setup requires to choose the maximum number of elements in the binary tree and the tolerance ϵ . The first parameter has to be high to tabulate as many values as possible, but a very high number of elements makes inefficient the search through the binary tree and occupies too much memory. As good compromise, 50 thousands elements were tabulated.

The tolerance value influences both the accuracy of the results and the computational time. To set up this value, a series of computations with different tolerances was performed in 2D meshes. Results are summarized in Figure 5, where a tolerance of 10^{-5} provides the best compromise in terms of accuracy and computational time. The resulting speed up factor as function of the used

tolerance is shown in Figure 6: when the number of cells is low the ISAT algorithm does not reduce consistently the computational time since there are few retrieves.

The speed up time drastically increases when the number of cells is higher: to compute a combustion process on the adopted 3D mesh on an Intel Xeon Dual-Core Core 1.8 GhZ with 4Gb Ram, direct integration takes about 30 days, while an ISAT computation with a 10^{-5} tolerance require 8 days: a high number of retrieves is achieved in this case because of the number of cells having similar compositions.

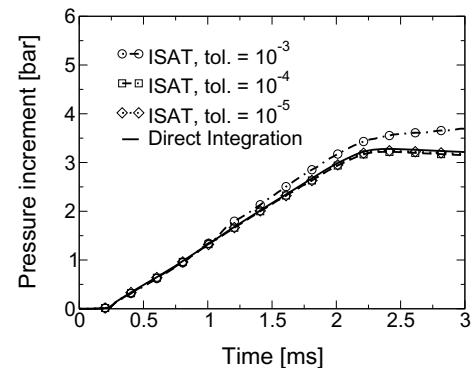


Figure 5: Pressure curves computed with Direct Integration and ISAT with different tolerances.

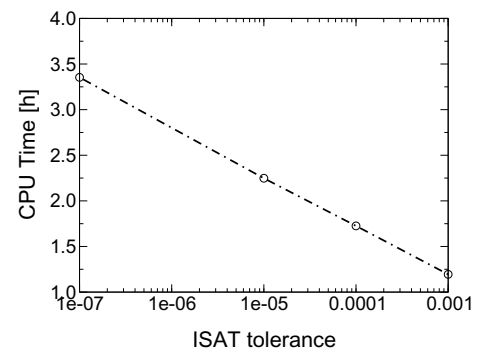


Figure 6: CPU time required as a function of the ISAT tolerance.

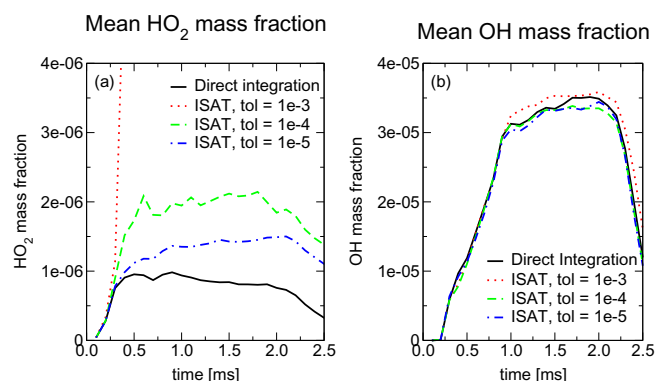


Figure 7: Influence of the ISAT tolerance on the mean HO_2 (a) and OH (b) profiles.

Finally, the influence of the ISAT tolerance on the species profiles is illustrated in Figures 7(a)-(b). The mean mass