Applying a Tabulated Chemistry Approach for the Calculation of Combustion and Emissions in Diesel Engines

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Abstract
It is generally acknowledged, that more details of the chemical reactions occurring in the flame front should be accounted for in the CFD simulations, but with increasing the number of species and reactions involved the associated CPU cost grows quickly beyond practical engineering time limits. Aim of this work is to increase computation efficiency by using a tabulation technique, without losing any accuracy. In order to achieve these goals, dedicated software solution for the generation of CFD look-up tables for advanced combustion models, is applied. Simulations were run for real life Diesel engine, for 5 different EGR levels. FGM results are showing very good match with measurements and direct calculation of the chemical reactions. The runtime for CFD simulations, including chemistry pre-processing, does only mildly increase with the number of species used in the reaction mechanism; simulations with 1000+ species have been realized within 20 hrs on 8 CPU cores.

1. Introduction

It is generally acknowledged that more details of the chemical reactions occurring during ignition and in the flame front should be accounted for in the CFD simulations to achieve higher accuracy. On the other hand the associated CPU cost grows quickly beyond practical engineering time limits with increasing the number of species and reactions involved. The FGM (Flamelet Generated Manifold) combustion model [1] overcomes this drawback and allows including state-of-the-art reaction mechanisms in CFD simulations at very practical CPU cost. This is achieved by a chemistry pre-processing technique that consists in precomputing the detailed combustion chemistry, storing the relevant data in a look-up table and interpolating from this table during the CFD simulations.

In this work, the AVL FIRE™ CFD software is used to compare predictions of the FGM model [2] and the detailed chemistry model to experimental data from a light-duty Diesel engine.

2. Combustion modelling approach

The combustion model has two main features: (i) chemistry tabulation based on auto-ignition trajectories of homogeneous fuel/air mixtures, computed[1] with detailed chemical reaction mechanisms and (ii) presumed-PDF turbulence-chemistry interaction (TCI) modelling. The FGM look-up tables are generated with AVL TABKIN™, a dedicated software program for the generation of CFD look-up tables for advanced combustion models. The look-up tables have up to 6 dimensions: pressure, fresh gas temperature, mixture fraction (Z), mixture fraction variance, progress variable and progress variable variance. The FGM combustion model is implemented in CFD code. A detailed chemistry model [3] is also available, named General Gas Phase Reactions (GGPR), and is used for FGM validation since it has been extensively used by various OEM end-users of AVL, for Diesel engine applications mainly. It allows reading an arbitrary number of species and reactions. For the calculation of chemical kinetics, a state of the art equation solver (Sundials library by LLNL) is coupled with an internal chemistry interpreter. An arbitrary number of chemical species and reactions can be applied. The chemical reaction scheme can be imported from any kind of 'Chemkin' compatible input file. The GGPR solution procedure supports massive parallelization. For boosting the performance in terms of calculation time, a multi-zone model is available, which collects computational cells with similar condition and solves the chemical reactions only once per group of cells. This has proven to be a very efficient way of calculating chemical kinetics. Additionally, 'In Situ Adaptive Tabulation' (ISAT) [4] model is available and a so called 'Dynamic Adaptive Chemistry' (DAC) [5] method, where the former one tabulates chemical reaction rates, which have been calculated once and provides the result if a similar condition is calculated again. The later method (DAC) performs an online sensitivity analysis and deactivates chemical reactions with small impact during a certain period. This leads to an additional reduction of calculation time especially before and after the main heat release takes place.

3. Engine simulations

The engine under investigation is a passenger car size diesel engine, which is equipped with a modern common rail injection system. The engine characteristics are provided in Table 1 below.

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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

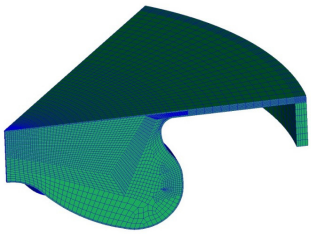

Fig. 1 Computational (sector) mesh

For this engine a large database of measured operating conditions exists. This database has been generated within a research project for the investigation of diesel surrogate fuels. All initial and boundary conditions have been closely checked in order to be consistent for the purpose of CFD validation.
In this work, an EGR sweep is considered for a low load operating point of 1000 RPM / 4 bar IMEP. The 5 EGR levels that were run are listed in Table 2.

Table 2. EGR levels for the 1000 RPM / 4 bar IMEP case

Case	**EGR**
A10146	11%
A10145	26%
A10142	39%
A10143	49%
A10144	56%

All cases have 4 injections: 2 pilot injection, 1 main and 1 post injection. For each load point, the injection timing is preserved for the EGR sweep, only the total amount of fuel is adjusted for each case. The repartition of the injected mass over the 4 injections is provided in Table 3 and the timing in Fig. 2 below.

Table 3. Injected mass repartition

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

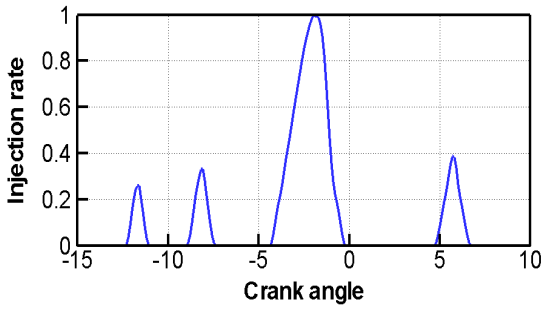

Fig. 2 Injection timing

4. Simulation analysis and discussion

As the purpose of this work is to compare both the FGM and GGPR combustion models to experimental data, the set-up of both models is kept as similar as possible. To this end, the following approach has been used:

1. The GGPR model was run with a reduced 45-species n-heptane mechanism [6];
2. The FGM look-up tables used the same 45-species mechanism;
3. The TCI model in FGM was not enabled, e.g. mixture fraction and progress variable variances were not considered;
4. The parameter settings for numerics and physical models were kept unchanged for all cases.

The pressure curves and derived apparent heat release rate (aHHR) are presented for the 1000 RPM / 4 bar case in Fig. 4, as measured and simulated with the FGM and GGPR combustion models. Global engine parameters like peak pressure, 10% fuel mass charge burnt (CA10) and 50% fuel charge burn (CA50) are distilled from Fig. 4 and summarized in Fig. 3.

The main findings from Fig. 4 are as follows, supported by the global parameters of Fig. 3:

1. Peak pressure magnitude is slightly under-predicted by the FGM model and over-predicted by the GGPR model (Fig. 3a).
2. Experimental aHRR profiles show that for low EGR the two pilots burn together around 714 CA. Then the aHRR of the main injection peaks around 720 CA and finally the post injection at 727 CA. When increasing EGR, the peaks in aHRR start merging more and more, until for 56% EGR the entire charge ignites and burns after the post-injection towards 727 CA. The increase in ignition delay is represented by CA10 in Fig. 3b.
3. The FGM model is quite able to follow this trend up to 49% EGR; for the 56% case, the ignition happens too early (Fig. 3b). The GGPR does not reproduce the experimental CA10 trend for lower EGR rates (Fig. 3b). The charge ignites and burns in all cases in two steps: after

the main injection the pilots+main charge burns and the post injection burns separately.

4. The experimental trend of increase of center of gravity CA50 (Fig. 3c) with increasing EGR is reproduced by both models, but the slope of the trend is under-predicted.

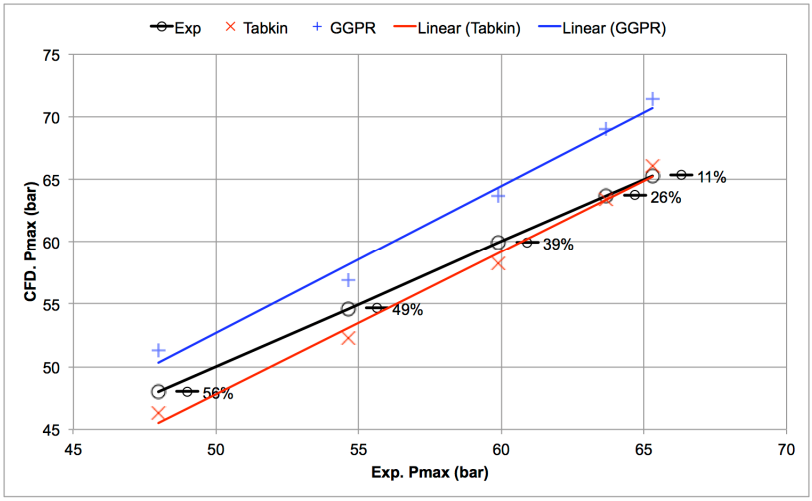

Fig. 3a Maximum pressure measured vs. simulated; percentages indicate EGR level.

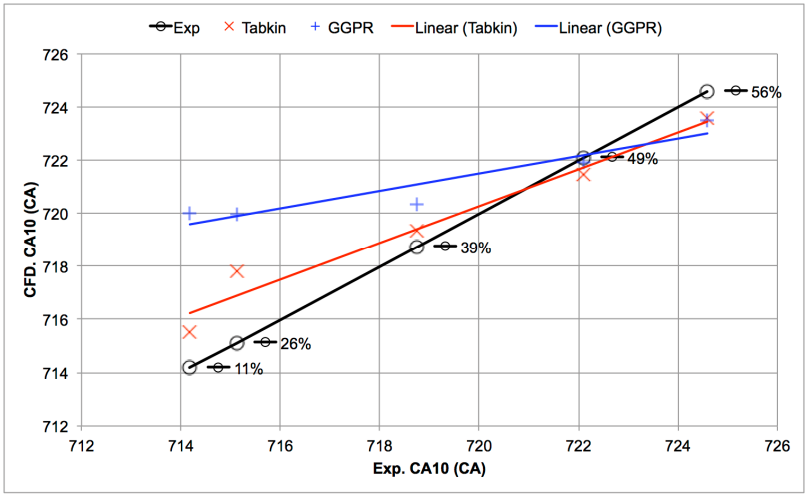

Fig. 3b CA10 measured vs. simulated

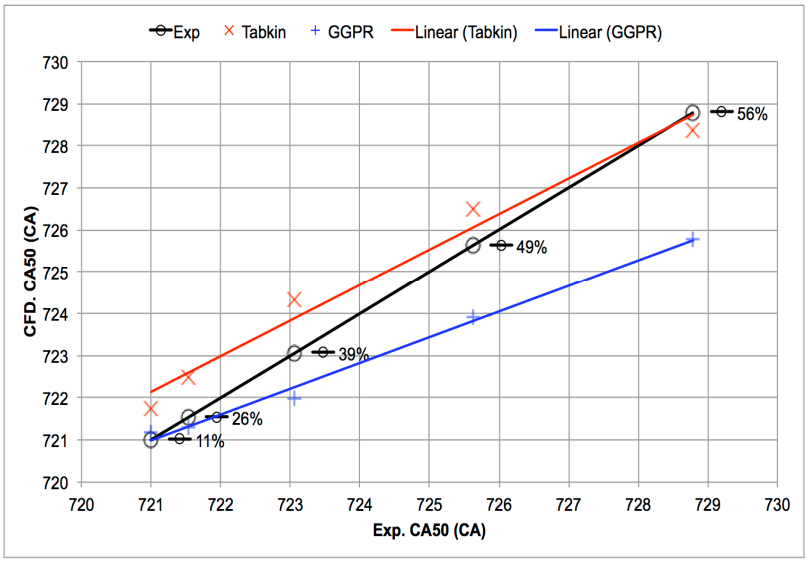

Fig. 3c CA50 measured vs. simulated

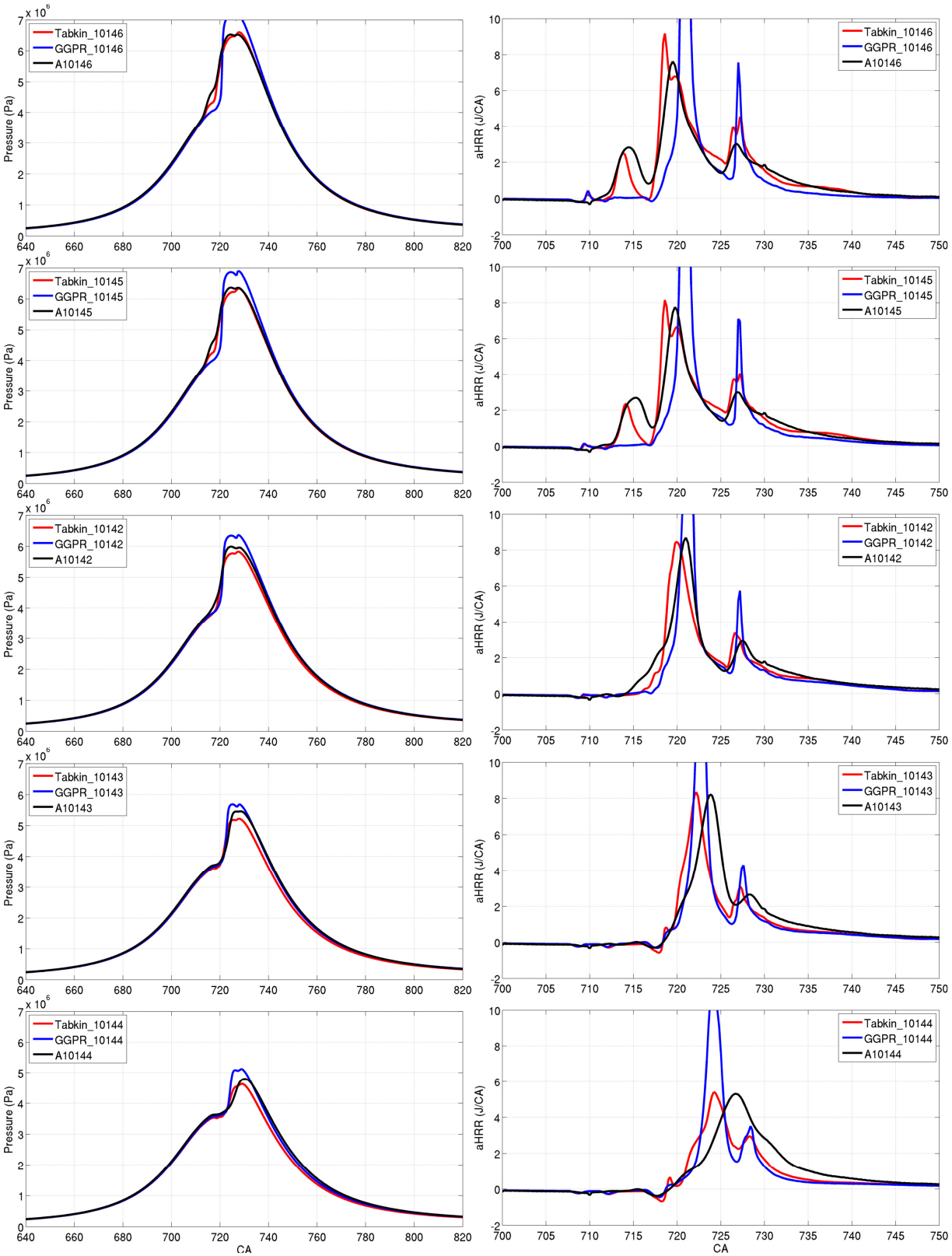

Fig. 4 Pressure (left) and apparent Heat Release Rate (right) as function of Crank Angle for 5 EGR levels, 1000 RPM / 4 bar BMEP case.

5. Emissions modelling approach

The soot emissions have been calculated by a kinetic soot model [6], which refers to a 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. The input for this model is a 'virtual fuel' species which is representative of not only the n-heptane, but all relevant fuel-related (radical) species.

For NOx, all NOx-related chemistry is computed during table generation. Then, the stored values of NO and NO_2 are retrieved during the CFD simulation.

The resulting NOx-soot trade-off is provided in Fig. 5 below. As can be observed, the trend observed in the experiment is well reproduced by the CFD simulation, identifying the maximum soot level at the 49% EGR case. Also the experimental trend of NOx decrease as a function of EGR is recovered; however, especially for the low EGR values the differences in absolute NOx values are substantial.

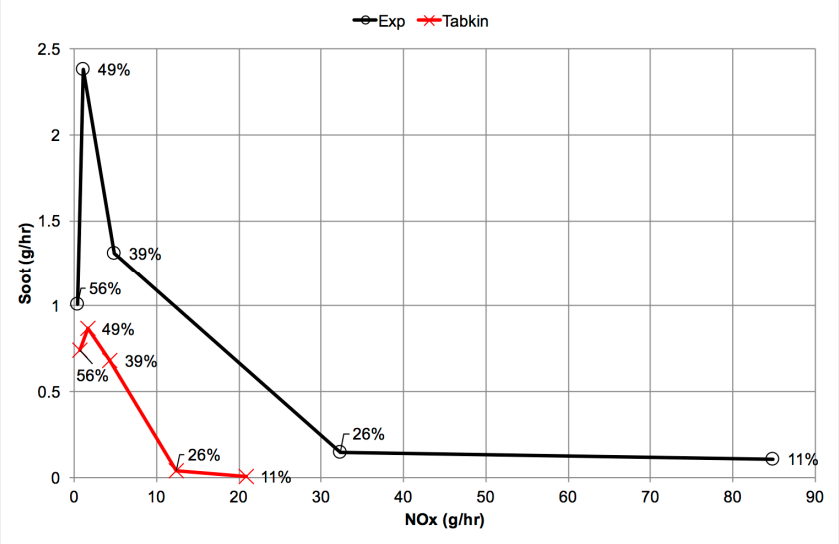

Fig. 5 NOx / soot trade-off measured vs. simulated; percentages indicate EGR level.

6. Conclusions

The FGM combustion model is compared to experimental data, together with the General Gas Phase Reactions (GGPR) combustion model. The FGM model relies on pre-calculated chemistry look-up tables which are then connected with CFD code. For a fair comparison, the same reaction mechanism is used in both combustion models and TCI is disabled in the FGM cases. An EGR sweep for a part-load case is investigated, with 5 different EGR levels. An injection strategy with 4 injections was used: 2 pilots, 1 main and 1 post.

Compared to the experimental data, peak pressure magnitude is slightly under-predicted by the FGM model and over-predicted by the GGPR model in nearly all cases. The experiments show that for low EGR, the combustion of the pilots and the main charge happens separately. With increasing EGR, the CA10 and CA50 also increase and the pilot and main charges eventually merge and burn together for maximum EGR of 55%. The FGM model is able to follow the CA10 trend up to 49% EGR, the GGPR does not reproduce the experimental CA10 trend. The CA50 trend is reproduced by both models, but the slope is under-predicted.

For the FGM case, the Soot-NOx trade-off is computed. For NOx, a direct look-up of the NOx values is used. For Soot, the FGM model is coupled to the kinetic soot model which is already implemented in the code. The experimental trend is that NOx decreases and soot increases with increasing EGR, but then for the maximum EGR level of 56% the soot level suddenly drops. This trend is well recovered by the FGM model; the differences in absolute NOx values are substantial for low EGR values and are topic of further research.

Overall, the FGM model shows improved predictive capability with especially capturing the trend of the staged combustion events with varying EGR percentages as well as the trend for Soot-NOx trade-off. With the addition of TCI and use of more detailed reaction mechanisms, FGM tabulation model offers a versatile toolbox for further improvement of CFD simulation predictivity for further engine design frontloading by simulation. Finally, the runtime for CFD simulations with FGM, including chemistry pre-processing, does only mildly increase with the number of species used in the reaction mechanism; simulations with 1000+ species have been realized within 20 hrs on 8 CPU cores.

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