Towards a Universal Combustion Model in STAR-CD for IC Engines:
From GDI to HCCI and Application to DI Diesel Combustion Optimization

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Gasoline Direct Injection (GDI) appears to be the most relevant way to improve fuel efficiency of SI engines. Homogeneous Charge Compression Ignition (HCCI) has also emerged as a viable alternative combustion process for Spark Ignited (SI) and Compression Ignited (CI) engines. The development of such engines is difficult. Every parameter, such as piston shape, injector inclination, or mixing process for example, has to be carefully adapted. CFD is a useful tool to understand the processes taking place in the combustion chamber and the correlation between parameters and, therefore, a way to support the design. However, CFD will require specific sub-models able to describe the spray and its evaporation, the mixing process and stratification, and the combustion process including auto-ignition.

A new combustion model developed in the GSM (Groupement Scientifique Moteurs including IFP, PSA and RENAULT) is implemented in STAR-CD: The Extended Coherent Flame Model-3Z (ECFM-3Z). This model is able to compute combustion for stratified charge in GDI engines complete with an auto-ignition model and a diffusion controlled combustion model. Therefore, it can compute all kinds of combustion regimes. The model is a development of the Coherent Flame Model (CFM), with the addition of thermal expansion effects and coupling with a burned/unburned gases conditional thermodynamic properties description. Application and validation of the model to DI Diesel combustion are shown in typical engine configurations.

In addition, the combination of the CFD tool with a multi-objective optimization tool ModeFrontier™ is applied to optimize the operating conditions for a DI Diesel engine.

1.0 INTRODUCTION

The development of CFD methodology for IC engine design represents a particular challenge due to the complex physics and mechanics, perhaps more than with any other widely-used mechanical device [1]. Improved understanding is essential to explore new solutions, reduce costs, and improve development efficiency. Although substantial advances have been made in all areas (turbulence, spray modeling, combustion, numerical methods, parallel computing, pre- and post-processing, etc.), there are numerous additional requirements to be met for it to become a design tool. The aim of this paper is to describe the recent developments in the multi-purpose CFD code STAR-CD [2] in the field of IC engine modeling with a special emphasis on DI Diesel engine combustion. An enhanced spray model and a new combustion model for GDI and Diesel engines is presented along with the optimization of a light duty DI Diesel engine using STAR-CD and the multi-objectives optimization tool ModeFrontier™.

2.0 THE MATHEMATICAL MODELS

2.1 THE SPRAY MODELS

The modeling of fuel injection processes is an essential part of DI Diesel engine simulation. The existing fully coupled stochastic Lagrangian-Eulerian approach used in STAR-CD [2] has been enhanced to avoid the necessity to empirically tune coefficients or other inputs of the spray model. These issues have been addressed in various ways in the enhanced implementation of the nozzle, atomization, and collision models.
2.1.1 The Nozzle Flow Model
The injection velocity, i.e. the velocity of the liquid fuel as it exits the nozzle and enters the combustion chamber, is one the most important parameters in a spray calculation. It strongly influences the atomization and break-up processes, the spray penetration, the inter-phase transfer processes, and the droplet-droplet interaction. The main feature of this model is the recognition of the creation of a separation/cavitation region emanating from the nozzle hole entrance. This results in the reduction of the exit cross-sectional area below its geometric value, which in turn increases the injection velocity. Depending on the pressure in the chamber relative to the critical pressure at which cavitation commences, and the length of the cavitation region, the model distinguishes three different flow regimes, i.e. the non-cavitating flow, the cavitating flow inside the nozzle, and the cavitating flow at the nozzle exit.

2.1.2 The Atomization Model
From the various built-in atomization models in STAR-CD, Huh’s [3] atomization model was chosen for this study. The characteristics and assumptions of this model are presented here. Huh’s model asserts that the two most important mechanisms in spray atomization are the gas inertia and the internal turbulence stresses generated in the nozzle. A conceptual picture can be described in two stages:

1. The turbulence generated in the nozzle hole produces initial perturbations on the jet surface when it exits the hole.
2. Once the perturbations have reached a certain level, they grow exponentially via pressure forces induced through interaction with the surrounding gas, until these perturbations become detached from the jet surface as droplets.

The model estimates the initial perturbations from an analysis of the flow through the hole and then uses established wave growth theory to represent the atomization process. The perturbation amplitude obeys a dispersion equation as derived by Taylor. The break-up rate of the produced parent droplets (obtained from the nozzle model) is calculated as a function of an atomization time scale and an atomization length scale. The diameter of secondary droplets formed from parent droplet break-up is estimated from a PDF. The minimum droplet size is calculated from Kelvin-Helmoltz instability theory. The atomization length and time scales are used to calculate the spray semi-cone angle. Finally, the estimation of initial velocity for each droplet is based on the assumption of equal probability of velocity direction within the spray cone.

2.1.3 The Enhanced Collision Model
There are a number of shortcomings in the original O’Rourke collision model that need to be addressed. These are that:

A. Computation time can be excessive.
B. No check is made to see if droplets are approaching each other.
C. Probability of collision is time-step dependant and can be high.
D. Parcels deplete too readily in coalescence.
E. Parcel density is based on the cell volume.
F. The method is inherently mesh dependant - only parcels in the same cell can collide.

These issues have been addressed in the enhanced implementation of the collision model as follows:

A. Reduced CPU time
The grouping process suggested by Schmidt and Rutland [4] has been implemented to improve the efficiency of the collision algorithm. This involves grouping parcels according to the cell in which they reside so that the parcels in any particular cell can be directly accessed. The new algorithm can give a speed-up of 30 times or more for some cases.

B. Additional checks on collision validity
Nordin [7] highlighted the fact that two prerequisites must be met if two parcels are to collide. The first is that the parcels must be traveling towards each other and the second is that the parcels’ relative displacements must be larger than the distance between them.

C. Deciding if a collision takes place

The new method implemented in STAR-CD is based on the work of Nordin [5], in which a probability is generated based on the minimum distance that will occur between the two parcels as they pass each other.

D. Timescale of coalescence

To limit the time-step dependency on coalescence, Aamir et al. [6] have suggested a limit on the number of droplets that can coalesce in a time-step by introducing a collision time-step. Therefore, the two probabilities are calculated and the number of droplets that will coalesce is taken to be the minimum.

E. Number density calculation

The need here is to redefine the number density in a mesh independent way. An attempt has been made to redefine the volume required for the number density based on the physical volume of both parcels involved in the collision. This is now based on a sphere plus cylinder volume.

F. Cell clustering

The enhanced collision model allows parcels that are not in the same cell to collide. Clusters are assembled by finding the cells immediately adjacent to a given cell. A second level of searching is performed to find the neighboring cells. Further cells could be added (if the user desired). Obviously the higher the number of levels, the longer the procedure will take.

2.2 THE COMBUSTION MODEL: ECFM-3Z

The ECFM-3Z model is a combustion model based on a flame surface density transport equation and a mixing model that can describe inhomogeneous turbulent premixed and diffusion combustion. This model is an extension of the ECFM [7] combustion model, previously implemented in STAR-CD and extensively validated for GDI applications. The idea is to divide the computational domain taking into account the local stratification. In the mixed zone, standard ECFM is computed, with an improved version of the post-flame chemistry model in the burned gases and an auto-ignition model in the unburned gases. The evolution of the mass included in the 3 mixing zones (Figure 1) are computed and modified with the help of a mixing model.

The general process of computation is as follows:
1. Computation of the mixed quantities
2. Calculation of the premixed combustion (ECFM + auto-ignition + post-flame)
3. Reconstruction of mean quantities

![Figure 1: Principle of the ECFM-3Z model](image)

2.2.1 The Auto-Ignition Model

The auto-ignition of the unburned mixture is computed over the mixed gases. The ignition delay is
computed through a correlation. Intermediate species integrate the advance in the auto ignition process. When the delay is reached, the mixed fuel is oxidized with a chemical characteristic time. The auto-ignited fuel is assumed to create a flame surface area: this is how it is coupled with the ECFM model.

2.2.2 The Regression Model
In order to be able to compute multi injection or local extinction, a simplified regression model has been introduced. This model just transfers burned gas quantities into unburned gas quantities when the local burned gas temperature is too low.

2.2.3 The Mixing Model
The first version of the mixing model is rather simple, based on the exchange with mean quantities. The amount of mixing is computed with a characteristic time scale based on the k-epsilon model. In this model we compute the evolution of two quantities: the unmixed fuel and the unmixed oxygen.

2.2.4 The Post-Flame Chemistry
The post-flame chemistry of the model is an improved version of the post-flame chemistry of the ECFM model. The major changes are the addition of a soot model and the introduction of kinetic oxidation of CO. The considered equilibrium reactions are:

\[
\begin{align*}
N_2 & \leftrightarrow 2N \\
O_2 & \leftrightarrow 2O \\
H_2 & \leftrightarrow 2H \\
2 \text{ OH} & \leftrightarrow O_2 + H_2 \\
2 \text{ H}_2O & \leftrightarrow O_2 + 2H_2
\end{align*}
\]

For the kinetic oxidation of CO we have:

\[
\text{CO} + \text{OH} \leftrightarrow \text{CO}_2 + H
\]

NO is calculated using the Extended Zeldovich mechanism.

2.2.5 The Soot Model
The Wisconsin ERC Soot Model is used for this first version considering a competing formation rate and an oxidation rate. The soot formation reaction uses an Arrehnius rate. The soot oxidation assumes two different reactive sites and the resulting oxidation rate is a function of soot properties (density and diameter) and kinetics parameters.

3.0 DI DIESEL COMBUSTION: MODEL VERIFICATION

Two different engine configurations were chosen to validate the described spray and combustion modeling.

ENGINE A: This is a typical light duty Diesel engine with displacement of 1.0 liter/cylinder equipped with a six-hole injector. The piston bowl shape is a Mexican hat profile with an open chamber as indicated in Figure 2. The swirl level is moderate and pilot injection is considered.

ENGINE B: This is also a typical light duty Diesel engine with a displacement of 1.80 liter/cylinder equipped with an eight-hole injector. The piston bowl is a re-entrant bowl type. (Figure 3)
3.1 GLOBAL CYLINDER DATA

Several cases were computed for both engines and global quantities were compared to experimental data.

A comparison between computed and measured in-cylinder pressure is presented in Figure 4 and Figure 5 in order to assess the accuracy of the computational model with respect to the prediction of global cycle averaged cylinder quantities. As it is shown, the predicted results show very good overall agreement with the measured values. In addition, the derivative of the in-cylinder pressure is compared to experiment for noise purposes. Figure 6 shows a typical comparison between calculated and measured pressure derivative. It can be seen that the pressure gradient magnitude is quite well predicted as well as its location in the cycle.

Figure 2: Bowl piston shape for Engine A

Figure 3: Bowl piston shape for Engine B

Figure 4: Comparison between calculated and measured cylinder pressure: Engine A, 50% Load, 2000 RPM

Figure 5: Comparison between calculated and measured cylinder pressure: Engine B, 100% Load, 1200 RPM

Figure 6: Pressure gradient history

Figure 7: Relative soot and NO formation trends at % EGR levels
3.2 EMISSIONS

The calculated global quantities of pollutant data serve as the basis for further assessment of the spray and combustion models’ behavior under engine operating condition parameter variations. This enables the study of the influence of injection timing, %EGR, etc. on soot and NOx formation. Figure 7 shows representative results of the relative soot and NOx formation trends for different %EGR levels.

4.0 DI DIESEL COMBUSTION: OPTIMIZATION

DI Diesel engine combustion chamber design (piston bowl shape, aspect ratio, etc.), fuel calibration, swirl, %EGR levels, etc., represent important independent parameters to optimize in order to meet the increasing demands of reduced fuel consumption and reduced emissions production. Even using a good optimization tool combined with test bench experiments is not sufficient, because the optimizer requires an instantaneous interaction between its algorithm and the new design configuration. This means: Stop the measurements. Apply the new design. Measure again. This is very time consuming and costly. Therefore, it is a good opportunity for CFD combined with an optimization tool to optimize and better understand DI Diesel combustion.

As an example, Figure 8 and Table 1 show the five different independent parameters used to obtain the optimum configuration that minimizes the soot and NOx levels and maximize the piston work. These parameters are the swirl level (SWIRL), %EGR level (%EGR), the number of injector holes (N_holes), the injection timing for the main injection (Tis), and the time between the end of the pilot injection and the start of the main injection (Dpi).

The simulation was conducted on a sector mesh and therefore, the angle of the sector was a function of the number of injector holes as well as the nozzle diameter. The injection pressure was maintained constant (the rail pressure). Table 1 summarizes the desired range of variation for the independent parameters as well as their respective increments. In Table 1, the number in parentheses represents the number of discrete tests (or runs) needed to scan each individual parameter. Therefore, if one would like to obtain all possible combinations, the total number of runs will be 38,016!!!

The purpose of an optimization tool is to find the optimum configuration with a minimum number of calculations, i.e. reduce the cost and effort.

![Image](image.png)

**Figure 8**: Injection profile

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Lower</th>
<th>Upper</th>
<th>Increment</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWIRL</td>
<td>0.3</td>
<td>2.3</td>
<td>0.2 (11)</td>
</tr>
<tr>
<td>%EGR</td>
<td>0</td>
<td>20</td>
<td>4 (6)</td>
</tr>
<tr>
<td>N_holes</td>
<td>6</td>
<td>12</td>
<td>2 (4)</td>
</tr>
<tr>
<td>TIS (CA)</td>
<td>350</td>
<td>380</td>
<td>2 (16)</td>
</tr>
<tr>
<td>DPI (CA)</td>
<td>10</td>
<td>50</td>
<td>5 (9)</td>
</tr>
</tbody>
</table>

**Table 1**: Independent parameters - range and increments
ModeFrontier™ was chosen as the optimization program. For the five independent parameters listed above, STAR-CD calculates the soot and NOx levels and the piston work during the closed phase of the engine cycle.

### 5 Independent Variables

- Swirl Level
- % EGR
- Start of Main
- End of Pilot – Start of Main
- N Holes Injector

### 3 Objectives

- Maximize Piston Work
- Minimize Soot
- Minimize NO

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**Figure 9:** Process flow in Frontier

Thanks to the input parameter flexibility of es-ice and PROSTAR, the pre and post-processor of STAR-CD, it is possible to easily achieve such a process flow with ModeFrontier including parameters affecting the geometry. The SOBOL algorithm in ModeFrontier is chosen to determine the original population. We limited ourselves here to only 10 runs. Then the MOGA (Multi Objective Genetic Algorithm) is chosen for the optimization process.

**Figure 10:** History chart for NO, soot, and piston work
One can see clearly that after the first 10 runs (design chosen randomly), the procedure is trying to minimize soot and NO and optimize the piston work. The result after 25 runs is summarized in Figure 11 and Table 2.

\[ \text{Figure 11: Optimization results after 25 runs} \]

<table>
<thead>
<tr>
<th>OPERATING CONDITIONS</th>
<th>Baseline</th>
<th>Optimized</th>
</tr>
</thead>
<tbody>
<tr>
<td>Swirl Level</td>
<td>1.0</td>
<td>1.86</td>
</tr>
<tr>
<td>%EGR</td>
<td>0.0</td>
<td>12.0</td>
</tr>
<tr>
<td>Injection Timing Main (ATDC)</td>
<td>12.0</td>
<td>-6.0</td>
</tr>
<tr>
<td>End of Pilot Injection – Start of Main</td>
<td>40</td>
<td>20</td>
</tr>
<tr>
<td>Number of Injector Holes</td>
<td>N</td>
<td>ident</td>
</tr>
</tbody>
</table>

In the process of optimization, it appeared that the soot is not reduced and probably one needs to execute more, or introduce another independent parameter like the injection pressure. However, because of the piston work increase, one can consider that the optimization is achieved just by reducing the amount of injected fuel. Therefore, the soot will be reduced by at least 10%. The maximum in-cylinder pressure was limited during the optimization process.

5.0 CONCLUSIONS

Presented in this paper are a new combustion model, the ECFM-3Z model, based on a flame surface density transport equation and a mixing model that can describe inhomogeneous turbulent premixed and diffusion combustion and substantial improvements of the spray model in STAR-CD. The combustion model is coupled with improved burned gas chemistry that allows CO, soot, and NOx formation calculations. After validating the model with several engine configurations and operating conditions, a method of optimizing DI Diesel combustion was presented in conjunction with an optimization tool.

6.0 REFERENCES


[2] STAR-CD V3.15 PROSTAR & es-ice are Trademarks of CD-adapco Group


