Modeling of Premixed SI-Engine Combustion
Using AVL FIRE – A Validation Study

M. Bogensperger, M. Ban, P. Priesching, R. Tatschl
AVL List GmbH
Advanced Simulation Technologies
Graz, Austria

INTRODUCTION

Numerical tools used for the analysis and optimization of SI-engine combustion chamber geometry and the related intake port design need to be capable of reflecting the impact of engine configuration and engine geometrical details on the flame propagation characteristics without the need for case-specific model parameter tuning. In addition, the increasing use of alternative fuels such as, e.g. ethanol and its blend with conventional gasoline fuel, compressed natural gas, hydrogen, etc. impose new challenges on the layout of present and future combustion systems and hence on the numerical tools employed for their simulation. Accordingly, the adopted combustion model needs to be capable of reflecting the impact of the different fuel physical and combustion properties onto the flame propagation and combustion characteristics.

In the present work the well known coherent flame modeling approach available in the CFD code AVL FIRE [1] is suitably extended to accurately predict premixed flame propagation characteristics in gasoline engine configurations over the relevant range of engine operating conditions. Furthermore, the model is adapted in order to reflect the impact of different fuel types on the local flame speed and hence on the overall combustion characteristics as well as on the pre-reactions in the end-gas leading to the onset of knocking combustion.

The resulting model is first validated for the premixed flame propagation process in a constant volume combustion chamber for variations of initial pre-combustion thermodynamic, charge composition and turbulence conditions by comparing the calculated flame size and chamber pressure evolution results with the corresponding experimental data. Then, the model is applied to the prediction of premixed SI-engine combustion in different passenger car engine configurations for WOT operating conditions. Model performance and predictive accuracy is assessed by comparing the calculated in-cylinder mass fraction burned data with their corresponding measured counterparts, indicating very good overall agreement for the investigated engine configurations and operating conditions.
COMBUSTION MODELING

For calculating IC-engine flame propagation and combustion, AVL FIRE adopts the ECFM/ECFM-3Z model suite developed along the lines of the coherent flame concept [2-5].

For modeling SI-engine premixed flame propagation the ECFM/ECFM-3Z model solves a transport equation for the flame surface density with source terms accounting for flame surface density production due to turbulent wrinkling of the flame and for flame surface density annihilation due to chemical reaction. In the present work the flame surface density production term is extended to be a function of the local in-cylinder turbulent flow conditions in order to more accurately account for turbulence/flame interaction effects typical for real SI-engine operating conditions.

The high temperature reactions inside the flame are modeled according to a largely reduced hydrocarbon oxidation scheme coupled with an equilibrium approach to capture the formation of O, H and OH radicals in the post-flame region. In its actual implementation the model fully accounts for equivalence ratio and residual gas inhomogeneities on the flame propagation characteristics, thus being able to also handle direct injection, stratified-charge combustion concepts.

Flame initiation is modeled based upon an extension of the original ECFM/ECFM-3Z spark-ignition model by introducing a refined treatment at the spark location for the local thermodynamic and charge-composition, flow velocity and turbulence conditions impact on the initial flame surface density.

The laminar flame speed information required in the coherent flame modeling approach is obtained in the present case from detailed chemical kinetics calculations and tabulation of the laminar flame speed data as a function of temperature, pressure, equivalence ratio and residual gas content (Figure 1). The detailed kinetics calculations and the tabulation of the laminar flame speed data are performed as a pre-processor step prior to the CFD calculation. The flame speed data tables once obtained for a specific fuel type are then available for any further calculation with AVL FIRE later on. A fast interpolation algorithm adopted for extraction of the tabulated flame speed information for its use within the coherent flame modeling approach ensures CPU efficient use of the detailed chemical kinetic information within the complex CFD calculation.

![Figure 1: Laminar flame speed data as a function of equivalence ratio and pressure for a) n-heptane and b) methane](image)

In the context of the coherent flame modeling approach adopted in AVL FIRE, the auto-ignition process in the end-gas region ahead of the main reaction zone is treated by solving a transport equation for an auto-ignition tracer species with the source term obtained from tabulated auto-ignition data. Similar to the flame speed tabulation approach, the auto-ignition tables are based upon detailed chemical kinetic calculations
of the fuel ignition behavior for the relevant range of pressure, temperature, equivalence ratio and residual gas content (Figure 2).

Figure 2: Auto-ignition delay time for n-heptane as function of temperature and pressure

**BASIC VALIDATION**

Validation of the ECFM/ECFM-3Z model extensions is achieved by comparison of the calculated and measured premixed flame propagation characteristics under idealized conditions. The configuration used in the present case is a constant volume combustion bomb, designed to closely reflect the SI-engine combustion process near TDC. The details of the combustion bomb and the experimental set-up are described in [6].

<table>
<thead>
<tr>
<th>Case</th>
<th>( T_{\text{init}} ) [K]</th>
<th>( P_{\text{init}} ) [bar]</th>
<th>( \phi ) [-]</th>
<th>Fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Baseline, quiescent</td>
<td>420</td>
<td>8.6</td>
<td>0.96</td>
<td>Propane</td>
</tr>
<tr>
<td>B Lean, quiescent</td>
<td>420</td>
<td>8.6</td>
<td>0.77</td>
<td>Propane</td>
</tr>
<tr>
<td>C Pressure, quiescent</td>
<td>420</td>
<td>4.3</td>
<td>0.96</td>
<td>Propane</td>
</tr>
<tr>
<td>D Temperature, quiescent</td>
<td>300</td>
<td>8.2</td>
<td>0.96</td>
<td>Propane</td>
</tr>
<tr>
<td>E Fuel, quiescent</td>
<td>420</td>
<td>8.6</td>
<td>1.0</td>
<td>Methane</td>
</tr>
<tr>
<td>F Higher turbulence</td>
<td>457</td>
<td>9.35</td>
<td>0.96</td>
<td>Propane</td>
</tr>
<tr>
<td>G Lower turbulence</td>
<td>447</td>
<td>9.15</td>
<td>0.96</td>
<td>Propane</td>
</tr>
</tbody>
</table>

Table 1: Combustion bomb - initial conditions

For validation of the tabulated laminar flame speed data obtained from the detailed chemical kinetics calculations and of the model extensions related to the flame surface density production term implemented in AVL FIRE, flame propagation under initially quiescent conditions as well as under swirling flow conditions are investigated. The quiescent test cases comprise of variations of mixture composition, initial temperature, pressure and fuel type, the swirling cases differ in terms of turbulence intensity, i.e. ignition timing after filling of the combustion bomb. The operating conditions of the investigated test cases are summarized in Table 1.

Figure 3 displays the impact of charge mixture composition and initial pressure and temperature on the flame evolution characteristics. The results clearly show the retarded
flame propagation speed when leaning the mixture (Case B) or reducing the initial charge temperature (Case D) when compared to the baseline case (Case A).

Figure 3: Combustion bomb – impact of mixture composition and thermodynamic initial conditions on flame size evolution

A reduction of the initial chamber pressure level, however, results in a slightly increased flame propagation speed (Case C). The good agreement between calculated and measured flame evolution characteristics for the charge composition and thermodynamic initial conditions clearly demonstrates the validity of the laminar flame speed tabulation approach used in the present study.

Figure 4: Combustion bomb – impact of fuel type on flame size evolution
In Figure 4 a comparison of the flame evolution speed is shown for a variation of the fuel type. It is clearly visible from the flame radius evolution results that the different laminar flame speeds of methane (Case E) and propane (Case A) lead to a remarkably different flame size evolution that is well reflected by the tabulated flame speed approach.

Figure 5: Combustion bomb – impact of turbulence intensity

Figure 5 shows a comparison of the calculated and measured chamber pressure traces for the cases with higher (Case F) and the lower (Case G) turbulence intensity levels. Though there are quite some uncertainties with respect to details of the experimental conditions prior to combustion initiation, the influence of varying turbulence intensity on the evolution of the chamber pressure trace is well reproduced by the AVL FIRE calculation.

ENGINE APPLICATION

In order to validate the flame speed tabulation approach, the extensions related to the detailed modeling of the flame surface density production term and the modifications of the spark flame initiation model under real engine conditions, AVL FIRE is applied to the calculation of premixed flame propagation in three different SI-engine configurations for a selected number of WOT operating conditions. The engines under consideration are typical representatives of modern 4-valve gasoline engines with a displacement of approximately 0.5 liter per cylinder. Bore and stroke of the four engines are in the range of 79-86 mm and 81-96 mm, respectively.

In order to provide proper boundary conditions for the combustion calculation the entire gas exchange and compressions strokes are calculated for the three engines under consideration. For that purpose the computational meshes are generated on the basis of available CAD data adopting the IC-engine meshing tool of AVL FIRE. Starting off from a baseline mesh generated at gas-exchange TDC, AVL FIRE automatically generates the whole set of moving meshes required to cover the entire engine cycle. The gas-side boundary conditions at the intake and exhaust flanges as well as the wall temperature boundary conditions are taken from 1D cycle simulation results adopting AVL BOOST.

In order to provide a proper data basis for model validation cylinder pressure measurements are performed for the relevant speed / load points for the investigated engines. In order to transfer the cylinder pressure data into mass fraction burned results used for comparison with the calculation results cycle simulations are performed adopting AVL BOOST.

Figure 6 presents a comparison of the calculated and measured mass fraction burned curves for the engines and related operating conditions under consideration. The calculated mass fraction burned results of the “Reference Case” are obtained by manual
model parameterization, the result data “Flow Quantities” are achieved by adopting the model extensions described above for an identical default set of model parameters for all cases. It can be seen from the results in Figure 6 that the calculated mass fraction burned curves obtained with the model extensions are in very good agreement with the measured data for all engine operating conditions under investigation.

![Graphs showing mass fraction burned for different engines and operating conditions](image)

**Figure 6:** SI-engines – calculated vs. measured mass fraction burned

**SUMMARY AND CONCLUSIONS**

The well known coherent flame modeling approach of the ECFM/ECFM-3Z model suite is suitably extended in the present work to optimize the accuracy in predicting premixed flame propagation characteristics in gasoline engine configurations for operation with conventional and alternative fuels. The extended models are implemented in the CFD code AVL FIRE and validated based upon the flame propagation process in a constant volume combustion chamber. Then the models are applied for the prediction of premixed
SI-engine combustion in different passenger car engine configurations for WOT operating conditions.

The model’s predictive accuracy is assessed by comparing the calculated mass fraction burned curves with the data extracted from cylinder pressure measurements and indicates very good overall agreement for the investigated engine configurations and operating conditions.

REFERENCES


