Auto ignition tabulation of N-Heptane in ECFM-3Z Combustion Model

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Abstract
Recent efforts of implementing autoignition tabulated data to AVL's code "FIRE" including cool flame ignition will be presented in this paper, focused on n-heptane as fuel. Current use of n-heptane in combustion simulations did not include the phenomenon of cool flame ignition, and taking it into account could improve simulations of combustion in CI engines, also with wider application spectrum. The methods and ideas behind implementing the cool flame data into the ECFM-3Z model will be presented, as well as a comparison between the temperature fields calculated with ECFM-3Z model on a simple 100 cell mesh and a standalone application using Chemkin package.

Introduction

Recent rapid advances in computer power lead to increased use of computational tools in engine design, significantly reducing the costs of simulations compared to laboratory engine experiments.

In addition, there has been significant improvement in the physical sub models used in engine simulations, and the enhanced accuracy has made the use of computational tools advantageous for generating a better understanding of the transient physical and chemical phenomena that occur in internal combustion engines. The goal of this study was to improve the prediction of diesel fuel auto ignition processes using tabulation approach to include the cool flame ignition phenomenon.

Flame development, power output and emissions formation are determined by the process of auto ignition in diesel IC engines and is dependent on chemical and physical processes. The first kind of processes is pre-combustion reactions of the fuel with air and residual gases, high temperature combustion and emissions formation. The main physical processes include atomization of liquid fuel, evaporation of fuel droplets and turbulent mixing of vapor with air. Rather than trying to simulate the complex behavior of diesel fuel itself the replacement fuel of choice is n-heptane due to its cetane number of approximately ~56, which is similar to that of ordinary diesel fuel.

Current diesel auto ignition model included in AVL code "FIRE" used a tabulated data acquired by running SENKIN calculations varying following initial parameters: temperature, pressure, air excess ratio and recirculating exhaust gas mass fraction. These values were used to simulate the exact ignition moment using a precursor variable in extended coherent flame combustion model. However, existing data provides only the main ignition delays, which is sometimes not accurate enough e.g. when running simulations in a low temperature region without taking cool flame phenomenon into account.

Chemistry Background And Numerical Approach

When studying the complex chemical mechanisms, it is possible to get a comprehensive insight of the chemical kinetics behind the phenomena of auto-ignition. N-heptane skeletal mechanisms (that include the main species and reactions) consist in general of 20-80 species with less than 250 reactions (Rente et al., 2001, Tanaka et al., 2003, Liu et al., 2004). These can further be simplified to 4-40 steps, but this approach (done by mathematical transformations) can cause the loss of physical meaning of the individual species (Peters et al., 2002). Initial tabulations for n-heptane were performed using small Golovitchev mechanism (Rente et al., 2001), but since the ignition delay acquired proved to be under predicted on the whole domain, it was rather used to determine the initial data simplifications to perform the tabulation using more complex mechanism.

The detailed n-heptane mechanism (of Curran et al., 1998) is intended to cover the entire range of conditions from low-temperature (600-900 K) pyrolysis and oxidation to high-temperature combustion. Several methods are used to reduce the chemical mechanisms to the size (skeletal or reduced models) appropriate for reasonable computation, based on sensitivity analysis, and others (the Quasi-Steady-State Assumption (QSSA), the Intrinsic Low-Dimensional Manifold (ILDM) approach or the Computational Singular Perturbation method (CSP)) (Valorani et al., 2007) . Also, one could base the survey on whether the mechanism simplification method is based on reduction of reactions (Bhattacharjee et. al, 2003) or reduction of species (Lu, 2005 and Pepiot, 2005.).

Recent studies show that, using auto-ignition delay as an optimization criteria, the Curran model could be reduced to 170-180 species (Najm et al., 2006), and some show improvement using even more reduced mechanisms (67 species and 265 reactions, Hewson 1997).

The chemical mechanisms used were:

- n-heptane:

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o Golovitchev with 59 species and 291 reactions,
o reduced Curran et al. with 159 species, 770 reactions.

In this study of auto-ignition phenomenon, a FORTRAN subroutine library CHEMKIN II was used assuming zero dimension and adiabatic changes. It is generally used to predict the time-dependent kinetics behavior of a homogenous gas mixture in a closed system using. There are many possibilities for the chemical kinetics problems that one may need to solve for various applications (Kee at al., 1989). The problems interesting to this study are:

- an adiabatic system with constant pressure,
- an adiabatic system with constant volume.

The energy equation for the constant volume case is

$$c_v \frac{dT}{dt} + v\sum_{k=1}^{K} h_k \dot{\omega}_k W_k = 0 \qquad (1)$$

with the mean specific heat of the mixture of $c_v = \sum_{k=1}^{K} Y_k c_{v,k}$, temperature T, specific volume v , enthalpy h_k and molar weight W_k . The net chemical production rate of each species results from a competition between all the chemical reactions involving that species. Each reaction proceeds coefficients are in the modified Arrhenius form (Lutz et al., 1989):

$$k_f = AT^{\beta} \exp\left(\frac{-E}{RT}\right) \qquad (2)$$

where the activation energy E, the temperature exponent β and the pre-exponential constant A represent the parameters in the model formulation.

Since monitoring the cool flame phenomenon was one of the main topics of this work, a way to create a general routine to be able to recognize both the cool flame and main ignition had to be created. A useful definition of the ignition delay time was obtained from Marakides (2004) which states that it could be presented as the time at which the temperature theoretically becomes infinite6 (the asymptote of the temperature curve – see Figure 1).

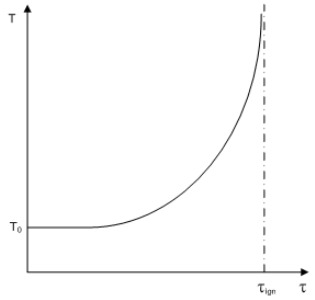

Figure 1. Simple theoretical ignition delay definition.

Several different criteria had to be implemented in the code to make it possible to get both the cool flame and main ignition delay times, as well as to filter out the misleading ignition-time candidates at the beginning of the calculation and around 1000 K. Fist approach was to use the temperature gradient which is checked at each time step and if an inflexion occurs the time is stored into a vector variable. If there is only one record in the vector variable at the end of the calculation, no cool flame ignition had occurred. In other case the first record is taken to be the cool flame ignition delay, and the last one is taken as main ignition delay. This approach provides good general and robust way to check for the ignition delay at real time but provides a problem when implementing in ECFM-3Z which will be discussed later.

Second approach is also rather commonly used, and assumes fixed temperature increase as an ignition criterion. In this approach the first ignition occurs when temperature increases for 10 degrees, after which the ignition watch is reset at the temperature inflexion point. At that point the second ignition is looked for, with the temperature increase of 30 degrees.

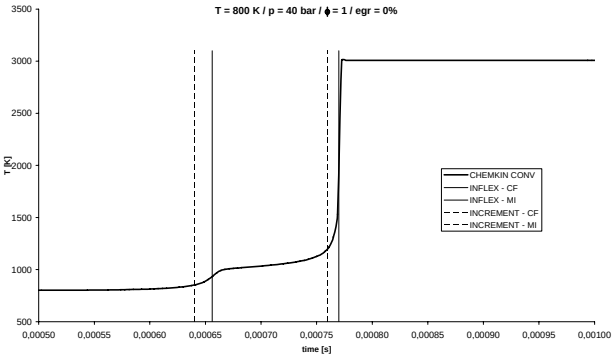

Figure 2. Comparison between the two ignition catching criteria

In the ECFM-3Z combustion model the ignition delay is computed either through a correlation or through an interpolation from tabulated values (the latter method is the one of the interest for this paper) (AVL FIRE, CFD solver v8.4, 2005). An intermediate species integrates the advance in the auto-ignition process for each time step in each computational grid cell (dependent on the cell's current pressure, temperature and mixture composition). When the delay time is reached, the mixed fuel is oxidized with a chemical characteristic time (see Figure 3 below).

Source term of the intermediate species is as follows:

$$\frac{\partial \overline{N}_I^M}{\partial t} = \overline{N}_{TFu}^M \Big|_M F\left(\tau_d\right) \qquad (3)$$

where M denotes the mixture zone, $\overline{N}_{TFu}^M$ represents fuel tracer in the mixture zone, and F is a function of delay time τ_d (tabulated value):

$$F(\tau_d) = \frac{\sqrt{\left(B^2 \tau_d^2 + 4(1 - B\tau_d) \frac{N_t^M \big|_M}{N_{TFu}^M \big|_M} \right)}}{\tau_d} \qquad (4)$$

where B is a constant set to 1s.

The same approach is used in modeling the cool flame ignition. In this case if intermediate species reach the tabulated value for cool flame delay (first combustion stage occurs), only a part of fuel should be consumed. This part is calculated from two more tabulated values, cool flame and main ignition heat release. The consumed fuel is calculated as a ratio of the heat releases from cool flame and main ignition. This approach is still an issue open to further discussion, but the results with the current setup seem very promising.

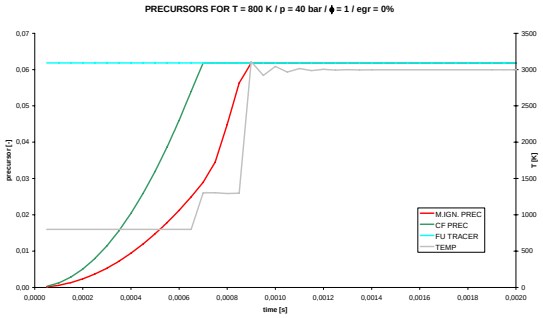

Figure 3. Fuel and intermediate species tracers development with temperature over time

The ignition data tables should provide the following data: cool flame ignition delay, cool flame heat release, main ignition delay and main heat release. Initial parameter ranges were taken out of existing tables (consisting of only main ignition delay times) and are shown in Table 1.

Table 1. Initial data for n-heptane tabulation using LLNL Curran reduced mechanism

Temperature [K]	650-750 K (20 K step), 790-1110 K (40 K) and 1500 K
Pressure [bar]	10 20 30 40 50 60 80
Equival. ratio [-]	0.3 0.5 0.7 1 1.5 3
EGR [%]	0 0.3 0.6 0.8

The data shown in above table is the final table done with several refinements (added two more points for pressure and one more point for equivalence ratio). The data is stored as ASCII values making it very easy to manipulate and refine before importing in AVL "FIRE" code.

Results and discussion

Initial data for more complex n-heptane mechanism calculations were obtained after observing some regularities and linear dependence of ignition data on temperature and pressure from the tabulation results with simple mechanism. Parameters held constant for each image were EGR mass fraction and air excess ratio. The idea behind this way of displaying data is to find the areas of near linear dependence of ignition delays on temperature and pressure to reduce the number of necessary calculations. Using the LLNL reduced mechanism (agreed on the fact that results it provides are close enough to the LLNL complex mechanism), acceptable number of calculations would be below 3000.The tabulated values shown on Figures 1-4 display clear dependence of ignition delay time on initial pressure and temperature, as well as the influence of EGR ratio for ethanol (less) and n-heptane (more). Also the ignition delay values for two n-heptane mechanisms are shown, with the Golovitchev data having been used to coarsen the initial values to get quicker tabulation time with more complex mechanism.

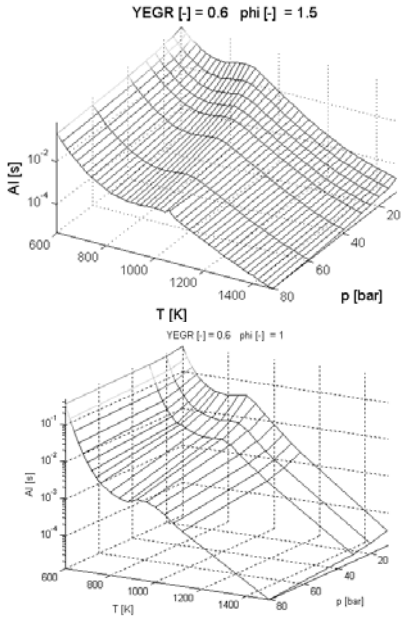

Figure 4. Comparison of one part of auto ignition databases created with Golovitchev (top) and LLNL Curran reduced (below) mechanism

Using the LLNL reduced mechanism, the result showed improvement regarding higher ignition delay times (thus closer to the ones using the most complex mechanism) as seen in Figure 4.

After the data had been imported into FIRE database, and ECFM-3Z ignition module modified to use it, a simple calculation case has been set up (Figure 5) to try and recreate the CHEMKIN calculation results using ECFM-3Z combustion model.

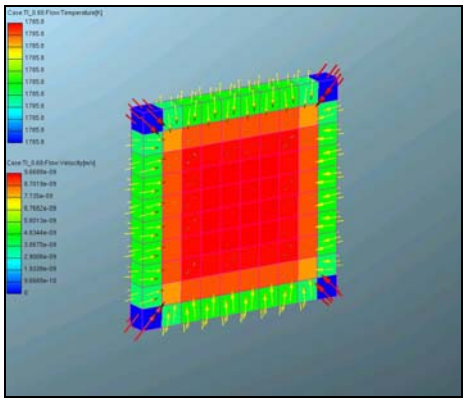

Figure 5. Calculation domain using FIRE

The Calculation domain set up was consisted of 100 cells (approx. 10cm by 10cm), time step was set to 2ms, end time was 2s, heat flux through the walls was zero, and the combustion model used was ECFM-3Z with modified two-stage ignition model.

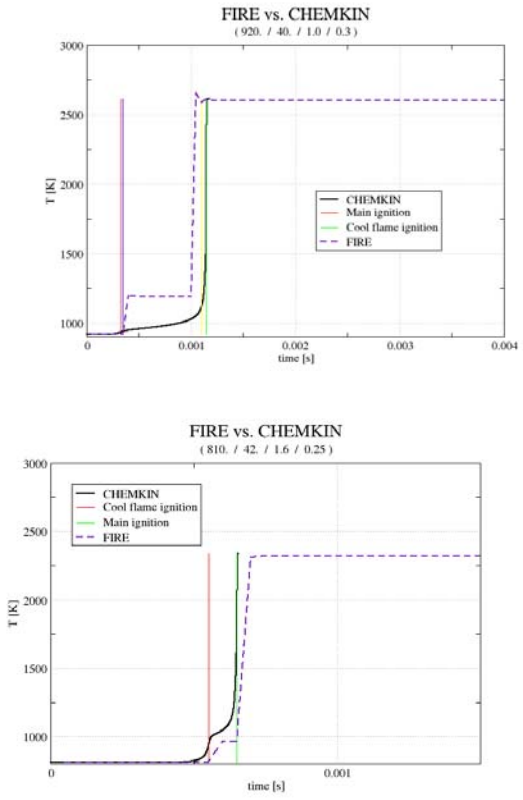

Figure 6. Comparing the CHEMKIN and FIRE calculation results

On the above images (Figure 6) one can see good agreement between the CHEMKIN calculated values, and the results obtained using FIRE solver. The second result image shows the need to use the second ignition criterion, because if the first one is used one gets later ignition times since temperature inflexion point (used as an ignition criterion) occurs at the 50% of the final temperature. Since the ignition delay time is used in ECFM-3Z model as a ignition start value, this yields the late ignition in some cases (with steeper temperature gradient).

The approach of using released heat for cool and main ignition for calculating the fuel consumption at cool flame ignition remains open to further investigation since it provides some over prediction in terms of cool flame temperature in some cases.

Finally, the overall approach proved itself to be rather reliable, robust for calculation and easy for post processing and data manipulation. There was successful attempt to use other mechanisms and fuels using the tabulation application (methane, ethanol), making it a promising tool for future use in ignition simulations on a wider scope.

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