

Modeling the ignition of sprays

C. Correa, B. Schramm, J. Warnatz

*Interdisciplinary Center for Scientific Computing (IWR), Im Neuenheimer Feld 368, 69120
Heidelberg, Germany*

email: correa@iwr.uni-heidelberg.de

Introduction

Ignition modeling is important in several industrial processes, an example of which is combustion in diesel engines. The simulation of the in-cylinder combustion depends on the accurate identification of the ignition delay time and the location of auto-ignition. As soon as the fuel is injected into the engine, low-temperature reactions occur leading to the formation of a radical pool. The concentration of this radical pool then increases during the ignition delay period due to chain reactions, eventually leading to ignition. Ignition chemistry can be accurately described by means of detailed chemical mechanisms [1] involving several hundred species and reactions due to the large number of radicals involved. The use of such reaction mechanisms in the simulation of complex 3-D flows is, however, prohibitively expensive because of the need to resolve other physical processes occurring, such as spray dynamics, turbulence, mixing, etc. Simplified ignition models however involve several unknown parameters which need to be fitted in order to give reasonable results. In this paper, a simplified ignition model is presented which is based on a detailed chemical mechanism. The main advantage of this model is that it is based on detailed chemical mechanisms and hence, do not contain parameters which need to be adjusted as the operating conditions are changed. This model was implemented in a modified version of the standard three-dimensional CFD code, KIVA III [3] which is capable of simulating two-phase engine flows. KIVA solves the three-dimensional Favre-averaged Navier-Stokes equations with a k - ϵ turbulence model. The spray dynamics was described by means of a discrete-droplet-model (DDM) where the probability distribution of the location, velocity, size and temperature of the droplets is solved for. This model contains with standard sub-models for collision, breakup, evaporation, etc. The breakup model used was a Kelvin-Helmholtz type wave model [4]. The liquid phase is coupled with the gas phase through an exchange of mass, energy and momentum. The resulting code was used to model a Caterpillar direct-injection diesel engine for which experimental results were available. Good agreement was observed between simulated and experimental quantities.

Ignition chemistry

n-Heptane was chosen as a model fuel for diesel as its cetane number is typical of a good diesel fuel and the reaction mechanisms are well known. At temperatures between 750-1150 K, autoignition of hydrocarbon mixtures show highly nonlinear behavior, showing the phenomenon of two-stage ignition and negative temperature dependence. Reaction mechanisms describing these phenomena hence contain several hundred species and reactions. The complete n-heptane reaction mechanism consists of 200 species involved in about 1200 elementary reactions. It was generated automatically using a computer code (LISP) [5]. This code is based on the fact that

only a limited number of different reaction types (e.g. alkane thermal decomposition) have to be considered, and the reactions and their rate coefficients can be formulated using simple rules [1]. The high temperature mechanism includes the following processes:

- Thermal decomposition of the parent hydrocarbon
- H-atom abstraction from alkanes and alkenes by H, O, OH, HO₂, etc.
- β -decomposition of alkyl radicals
- Isomerization of alkyl radicals

The low temperature reaction mechanism includes the following processes:

- Two consecutive O₂ additions to alkyl radicals
- Isomerization of alkylperoxy and alkylhydroperoxy radicals to cyclic structures
- OH elimination following this rearrangement
- β -decomposition of O=RO, C=RO, O=R and alkenyl radicals

This detailed n-heptane mechanism has been tested and proven to successfully predict two-stage ignition (as shown in Figure 1) and negative temperature dependence (as shown in Figure 2).

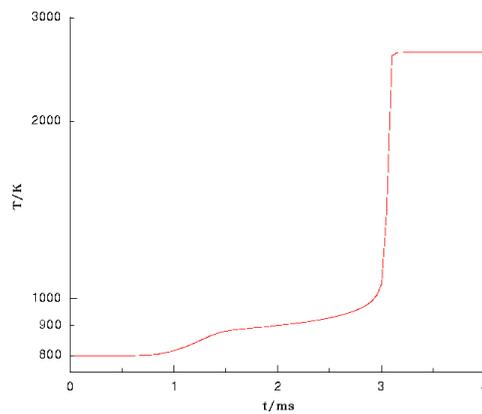


Figure 1: Two-stage ignition for a stoichiometric n-heptane-air mixture, isobar with $p = 15\text{bar}$, adiabatic, $T_0 = 800\text{ K}$

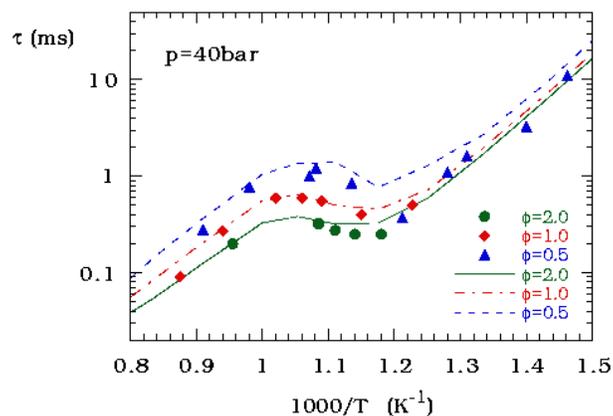


Figure 2: Comparison between calculated and measured ignition delay times for a range of equivalence ratios (lines: simulation, symbols: experiments) [1]

Ignition modeling

As discussed in the previous section, a detailed mechanism containing about 200 species involved in about 1200 elementary reactions was proven to accurately reproduce ignition delay times in a heptane-air mixture for a range of equivalence ratios. The use of such models in practical 3-D simulations is impractical due to the large number of transport equations involved. However, the development of the radical pool can be tracked with the help of one representative species, as the runaway of the species occurs simultaneously during ignition. This species should have the property of having a near zero concentration during the ignition delay period and showing a sharp increase at ignition, and CO was shown to possess these properties [2]. Thus, only one transport equation needs to be solved for the CO concentration, which looks like

$$\frac{\partial \bar{\rho} \tilde{Y}_{CO}}{\partial t} + \text{div}(\bar{\rho} \tilde{u} \tilde{Y}_{CO}) = \text{div}(\bar{\rho} D_T \text{grad}(\tilde{Y}_{CO})) + \bar{\rho} \tilde{Y}_{CO}^C \quad (1),$$

where $\bar{\rho}$ is the Reynolds-averaged density, \tilde{Y}_{CO} is the Favre-averaged CO mass fraction, \tilde{u} is the velocity vector, D_T is the turbulent diffusion coefficient and \tilde{Y}_{CO}^C is the mean source term due to chemistry. In order to get the laminar chemical source term, several trajectories were traced in homogeneous reactors for several values of the mixture fraction (ξ), temperature (T) and pressure (p) using detailed chemistry. Reaction rates of CO were then tabulated as functions of ξ , T , p and the CO mass fraction itself (Y_{CO}). In order to use it in turbulent flames, it needs to be integrated over a probability density function (pdf). In this paper, a presumed pdf method is used, where the shape of the pdf is assumed *a priori* and the parameters of the pdf are calculated from the moments of the variable (its mean and variance). The mean source term is now given by

$$\tilde{Y}_{CO}^C = \int \dot{Y}_{CO}^C \cdot P(\xi, p, T, Y_{CO}) \cdot d\xi \cdot dp \cdot dT \cdot dY_{CO} \quad (2).$$

Assuming negligible pressure fluctuations, and assuming statistical independence of the variables, the pdf can be split into the product of one-dimensional pdfs, i.e.,

$$\tilde{Y}_{CO}^C = \int \dot{Y}_{CO}^C \cdot P(\xi) \cdot P(T) \cdot P(Y_{CO}) \cdot d\xi \cdot dT \cdot dY_{CO} \quad (3),$$

and beta functions [6] were used for the three pdfs.

Results

The above ignition and chemistry models were implemented in KIVA III and were used to model a Caterpillar engine, for which experimental results were available [7]. The engine specifications are listed in Table 1. Since the combustion chamber geometry and the six-hole injector configuration is symmetrical, the entire computational domain was divided into 6 equal sectors, and the computational domain actually simulated was one-sixth (60°) of the total chamber. The numerical mesh used contained about 27,000 cells at BDC and about 9,800 cells at TDC. Experimental data were available for 5 different injection timings. Figure 3 shows the behavior of the representative species (CO) during the ignition delay period for the case with SOI -7° ATDC. Its concentration remains near zero during this period, and shows a sharp increase indicating ignition. Figure 4 shows the ignition location relative to the spray. The size of

the droplets correspond to the actual spray droplet sizes and they are colored according to temperature. As can be seen, ignition occurs at the edge of the spray in the lean region due to the higher temperatures present. These trends were observed in all the cases simulated (all the injection timings).

Bore	137.16 mm
Stroke	165.1 mm
Conrod length	263 mm
Piston crown	Mexican hat
Engine speed	1600 rpm
Number of nozzle orifices	6
Injection timing	-7, -4, -1, 2, 5° ATDC
Duration of injection	19.75°
Fuel injected	0.168 g/cycle

Table 1: Caterpillar engine specifications

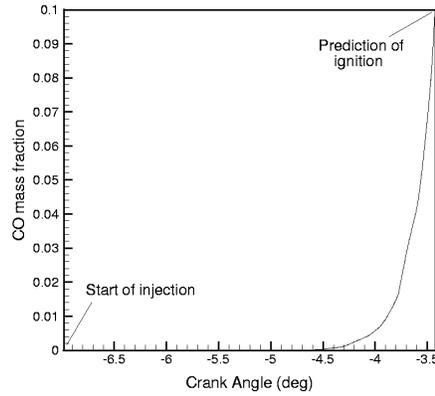


Figure 3: Maximum value of the CO mass fraction in the cylinder as a function of crank angle starting at injection till ignition (SOI: -7° ATDC)

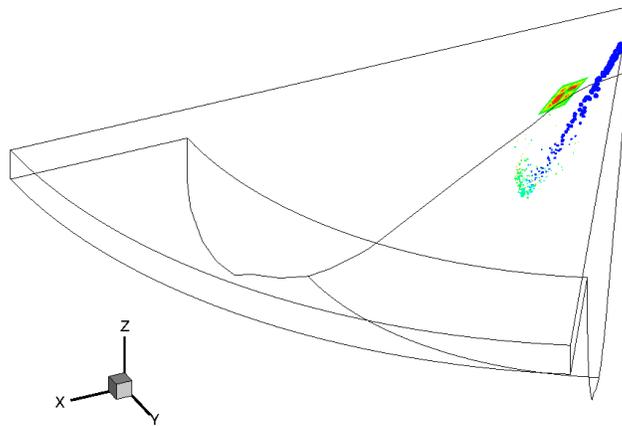


Figure 4: Location of ignition relative to the spray (SOI: -7° ATDC)

A comparison between experimental and simulated pressure curves for two of the injection timings are shown in Figure 5. A good comparison is seen for all the cases. It must be emphasized that no parameters were changed between any of the cases.

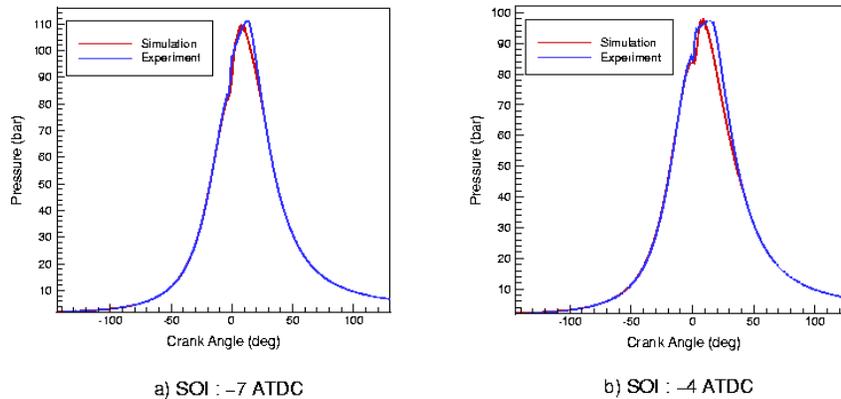


Figure 5: Comparison between experimental and simulated pressure for (a) SOI: -7° ATDC, (b) SOI: -4° ATDC

Conclusions

An ignition model based on detailed chemistry was implemented in a modified version of KIVA III and used to simulate a direct injection Caterpillar engine. The detailed chemical mechanism was verified against experimental data. The ignition model used a representative species to track the radical pool development during the ignition delay period and to predict the ignition location and timing. The model was coupled with a presumed pdf method to obtain mean chemical terms. The advantage of this model is that no parameters need to be adjusted for different engines and operating conditions. Good agreement was seen between the experimental and simulated pressure curves.

References

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