Flamelet Generated Manifold Strategies in Modeling of an Igniting Diesel Spray

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A study is presented on the modeling of fuel spray combustion in diesel engines. The objective is to model igniting diesel sprays with the detailed chemistry tabulation method FGM (Flamelet Generated Manifold). The emphasis is on the accurate prediction of auto-ignition as well as the steady combustion phase using one consistent approach.

Introduction

Due to ever increasing demands from emission legislation ($\mathrm{NO_x}$ and soot), fuel economy ($\mathrm{CO_2}$) and fuel flexibility (bio-fuels) diesel engines become more and more complex. Therefore, conventional engine design approaches that rely on prototype development become too time-consuming and expensive. The development of predictive and efficient computational tools would represent a significant step forward in the ability to rapidly design high efficiency, low emission engines [1].

Modern diesel engine technology unequivocally applies liquid fuel injection with high pressure, that forms a non-homogeneous mixture leading to relatively high levels of soot. Modeling this process is extremely difficult due to the complex phenomena occurring during fuel injection and combustion. A direct approach (DNS) is unviable and advanced, so accurate and fast sub-models are needed to apply it in engine design.

Recently, efforts to accurately and efficiently model diesel spray formation resulted in a suitable model to compute the mixture formation [2]. And a first application of the FGM method to a diesel spray proved that experimentally observable phenomena like auto-ignition and flame lift-off can be successfully predicted with this method [3]. The objective of this study is to compare the spray ignition behavior for different manifold types.

FGM Strategies

The FGM approach combines the flamelet concept with a manifold method by using mixture fraction Z and progress variable PV to parameterize the combustion process [4]. Recently, the application of the FGM method proved to be able to predict auto-ignition and flame lift-off for a diesel spray simulation in engine-like conditions. However, different 'generators' can be chosen to fill the unsteady flamelet region, which may influence the final results in terms of for instance ignition delay time and combustion behavior.

FGMs can be generated in many ways. For stationary flames, there is a classical way with steady flamelets only, where a sequence of steady flames with strain rates varying from a low value (close to equilibrium) to the quenching value is computed. An illustrative example of the "accessible" space in Z-PV is shown in Figure 1, see the gray area between the solution for the lowest strain rate and the solution at which the strain rate reached its maximum before extinction.

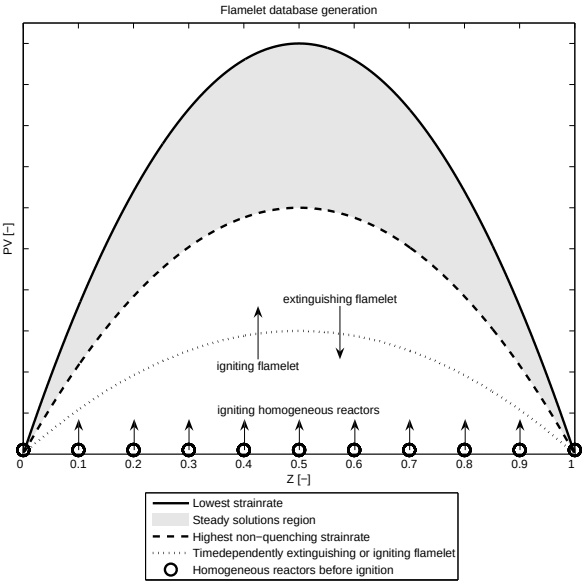

Figure 1: Ways to extend a stationary database

Diesel combustion is characterized by auto-ignition, so to cover this aspect the table should also contain information in the area beneath the quenching strain rate solution. Several ways exist to fill this gap in the Z-PV plane. One way is to solve a time-dependent flamelet with a higher strain rate than the highest possible non-quenching strain rate. In this way the flame is forced to extinguish and in the mean time data are sampled to fill the gap. Another approach, that is more appropriate for this study, is solving time-dependent flamelets from a mixed, but non-reacting initial state. The ignition behavior is followed in time until a steady flame is reached. A third possibility is to reproduce ignition of mixtures covering the entire Z-space with homogeneous reactor auto-ignition calculations [5]. All three methods to fill the Z-PV gap are depicted schematically in Figure 1.

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Preliminary Results

Due to the unsteady nature of a diesel injection event, ignition modeling is at least as important as combustion modeling. Following the FGM approach, besides combustion, ignition should be covered inherently. But the result depends on the way the FGM is generated. The extinguishing flamelet approach is applied and does not lead to ignition of the spray. Instead, only local temperatures slightly above the initial ambient temperature are found, and the source of the reaction progress variable is not big enough to end in total ignition within a few milliseconds. However, a FGM constructed with an igniting flamelet or homogeneous reactor database does result in auto-ignition of the whole spray in short time. Therefore, in this paper only the results of the igniting flamelet and homogeneous reactor approaches are presented.

In this study non-premixed flamelets for a counterflow setup are solved with CHEM1D [6] and the homogeneous reactor simulations are performed with XCCI [7]. Both are dedicated codes, developed at the Eindhoven University of Technology, for one-dimensional laminar flames and single/multi-zone reactors, respectively. The heptane databases are calculated at constant pressure, making use of a reduced n-heptane mechanism [8].

Here the Z definition of Bilger [9] is adopted and PV is chosen as a combination of CO_2, CO and CH_2O mass fractions. The created laminar manifolds parameterized with the mixture fraction Z and reaction progress variable PV are depicted in Figure 2 for the flamelets case (ignition at strain rate 500) and in Figure 3 for the homogeneous reactors case. In these two figures the contours of the PV source is plotted. Some major dissimilarities can be observed when these figures are compared. Firstly, the position of the maxima of the sources is different, and secondly the values of the maxima differs with a factor of approximately 30. The igniting flamelet database shows high source terms in the region $0.05 < Z < 0.15$, whereas the homogeneous reactor database shows a much wider highly reactive region extended to fuel richer compositions $0.05 < Z < 0.3$. And the PV source terms in this highly reactive region are higher than the ones of the flamelet database. From this comparison one can conclude that convection and diffusion, which are not present in the homogeneous reactor case, have a large impact on the ignition behavior in Z-PV space.

Eventually, when the laminar manifolds are integrated with presumed β-PDF functions, the dissimilar manifolds also result in different auto-ignition position and time of a 3D turbulent spray. Due to the higher PV sources, the homogeneous reactors lead much faster to ignition than the flamelet case. And because of the position of the high source terms, the ignition spot in the homogeneous reactors case is at a more fuel rich region ($Z > Z_{stoich}$) than in the flamelet case ($Z \approx Z_{stoich} = 0.064$). These are also visualized in Figure 4 by means of temperature contours at the moment that an ignition spot increases with 50 K above the ambient temperature, prior to an exponential increase to temperatures above 2000 K. So far, when compared with literature [10, 3] the results with the igniting flamelet manifold gives more realistic predictions.

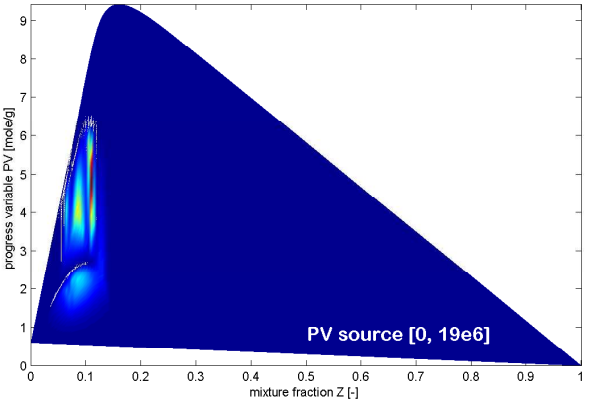

Figure 2: Igniting flamelet manifold. PV source as function of Z and PV.

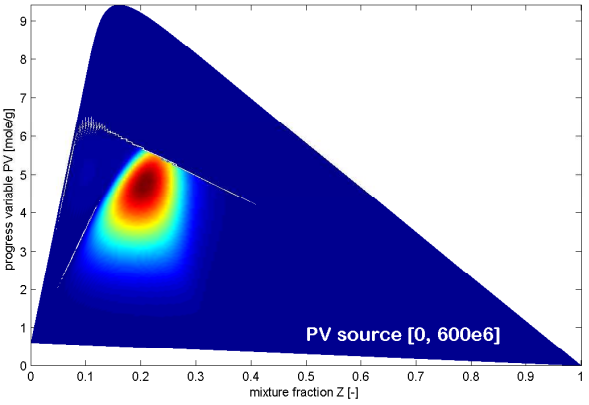

Figure 3: Homogeneous reactors manifold. PV source as function of Z and PV.

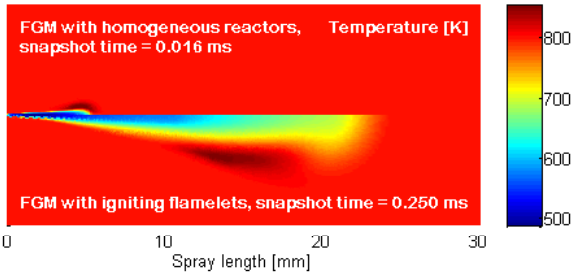

Figure 4: Temperature contours. At start of injection the time is 0 ms and the ambient temperature is 800 K.

Outlook

In the quest for a generic approach to model the important chemistry related characteristics in diesel sprays, the observed dissimilarities in auto-ignition prediction between the FGM tabulation strategies are to be investigated. This is going to be done with 0D and 1D laminar simulations to exclude the possible influences of turbulence modeling and/or complicated interactions within the used Fluent framework. Especially the effects of progress variable choice and the choice of strain rate at which the igniting flamelet is calculated are points of interest.

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