Modeling Diesel Spray Ignition Using Detailed Chemistry with a Flamelet Progress Variable Approach

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Introduction

A well-established way of modeling diffusion combustion is the representative interactive flamelet (RIF) concept [1]. In the RIF concept the computational fluid dynamics (CFD) code performs the flow calculations, and the ignition and combustion is calculated by an unsteady flamelet code handling the combustion chemistry, which interacts with the CFD code. The interaction is achieved by means of two additional scalars, the Favre averaged mixture fraction and the Favre averaged mixture fraction variance. This method does not require the transport of species, as the combustion chemistry is handled by the unsteady flamelet code. In the RIF concept, considering local effects such as local turbulence and other inhomogeneities on the CFD grid cell level (a global value for the scalar dissipation rate is used in the single-RIF model) is restricted, as this would require one flamelet in each cell. In modeling Diesel engines, a very high number of cells is required to resolve the combustion chamber geometry. Having a flamelet in each cell would impose immense requirements on computer memory and CPU time if a detailed chemical mechanism is employed.

There are however other ways of obtaining information in a flow calculation on the progress of an ignition or combustion process, for example by means of a progress variable. Zhang et al. [2] advocate the use of a normalized time variable describing the ignition process, based on an (in mixture fraction space) integrated major species. By means of an unsteady flamelet library, for the source term of the normalized time variable and the chemical heat release, the autoignition and flame propagation is predicted for a turbulent autoignition problem. Pierce and Moin [3] propose for the use in large eddy simulations (LES) a steady flamelet approach, but using a flamelet parameter based on a reactive scalar in addition to the scalar dissipation rate for the mixture fraction. Ihme et al. [4] discuss the applicability of this model when predicting local extinction and re-ignition. Kronenburg and Papoutsakis [5] suggest, for the conditional moment closure (CMC) method a CMC with sensible enthalpy for the chemical reaction rate terms to accurately model extinction and re-ignition .

In this work, an unsteady flamelet library for a flamelet progress variable, based on enthalpy, is used to model autoignition under Diesel engine relevant conditions. Our approach is, as in [2], based on the assumption that a normalized time variable, an integrated flamelet progress variable, uncoupled from the mixture fraction space, can be used to describe the flamelet state during ignition. We base, however, this integrated progress variable on sensible enthalpy. This implies also that all information of the ignition process, in each cell in the CFD grid, is described by this scalar. As in [2] we store the source terms of the integrated flamelet

progress variable in an unsteady flamelet library, but instead of storing the chemical heat release, an expression for the enthalpy as a function of temperature and mixture fraction is stored. This means that the CFD code only has to transport the Favre averaged integrated flamelet progress variable in addition to the Favre averaged mixture fraction and Favre averaged mixture fraction variance. The source term for the integrated flamelet progress variable is obtained from the library as a function of amount of EGR (exhaust gas recirculation), pressure, oxidizer temperature, scalar dissipation rate, and the integrated flamelet progress variable itself. As an expression for enthalpy as a function of the integrated flamelet progress variable, EGR, pressure, oxidizer temperature, mixture fraction, temperature in mixture fraction space and mixture fraction is stored in the unsteady flamelet library, the temperature in each cell can be calculated using an iterative procedure, provided that the Favre averaged enthalpy is transported in the CFD code, and by using a beta-probability density function in mixture fraction space. By transporting the Favre averaged enthalpy, and using an iterative procedure to calculate the temperature in each cell, local effects such as heat losses to the walls can be considered. Furthermore, this method allows considering local turbulence effects since the local scalar dissipation rate is used.

Calculations and Results

An unsteady flamelet library was calculated using a chemical mechanism for n-decane containing 101 species and 841 reactions. The flamelet library calculations were performed for a spray-bomb case at a pressure of 80 bar, a fuel temperature of 298 K, and oxidizer temperature of 1060 K, for one case without EGR and one case with 20% EGR. The scalar dissipation rate was varied in an interval of 0.5-1000 1/s in the flamelet library calculations. This set-up corresponds to approximately the conditions at ignition in a low-load Diesel case with late injection.

The flamelet library is built by first using a steady flamelet code to calculate the stationary profiles for each case in EGR-pressure-oxidizer temperature-scalar dissipation rate-space. This is followed by unsteady flamelet calculations. The unsteady flamelet code is initialized, in mixture fraction space, with a profile of a not ignited flamelet. The ignition process of the flamelet is traced and parameterized using the integrated flamelet progress variable. Finally the flamelet library is compressed and a subroutine for use in CFD codes is written.

As a first test of this method, STAR-CD was coupled with the unsteady flamelet library model to perform the 2D-flow calculations. The same set-up was used for the single-RIF [6] coupled with STAR-CD calculations, which constitute the reference calculations. Note however that the chemical mechanisms for n-decane in both models differ slightly.

The maximum temperature for the case without EGR is shown in Figure 1. It is observed that ignition occurs slightly earlier when using the unsteady flamelet library model. There are however only slight differences in the maximum temperature after 0.4 milliseconds. The maximum temperature for the case with 20% EGR is shown in Figure 2. Here we see that ignition occurs later as expected using the unsteady flamelet model, which is not seen, in this case, using the RIF method. The maximum temperature predicted by both models, is lower than in the case without EGR. Also here we notice that there are only slight differences in maximum temperature after 0.5 milliseconds. The more detailed information of the

autoignition process seems not to influence the further development of the turbulent diffusion flame. Maximum temperature is used since the volume of the spray bomb is so large that the average temperature is not useful as a measure for the ignition timing. When analyzing the results of the 2D calculation it was observed that the ignition occurs at the edge of the spray.

The 2D temperature profiles for the 20 % EGR calculation using the unsteady library approach and the single-RIF after 1 millisecond and 2 milliseconds are shown in Figure 2. It can be observed that, the profiles are virtually identical.

Conclusion

An unsteady flamelet library for the integrated flamelet progress variable containing an expression for enthalpy was used to predict autoignition under Diesel relevant conditions. Using this approach we are able to resolve local effects such as local turbulence and heat losses to the walls on a CFD grid-cell level. In a first test case, in which STAR-CD was coupled to the unsteady flamlet library, we have shown that the results using the proposed model are virtually identical to results obtained with the single-RIF model after autoignition.

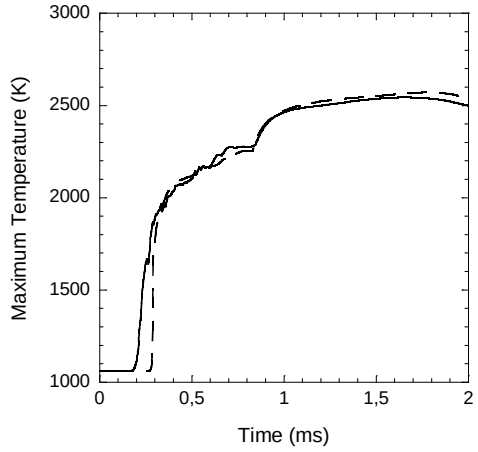

Figure 1. Maximum temperature for the unsteady flamelet library approach (solid line) and RIF (dashed line), 0% EGR.

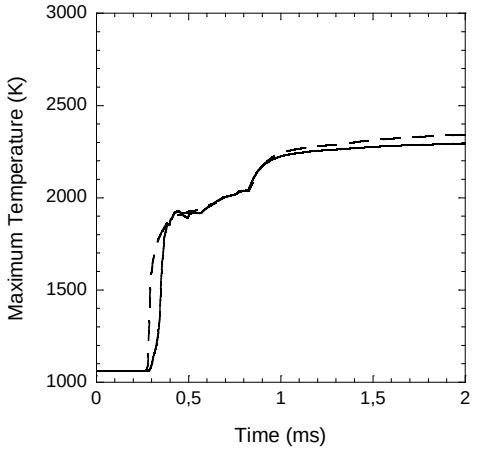

Figure 2. Maximum temperature for the unsteady flamelet library approach (solid line) and RIF (dashed line), 20% EGR.

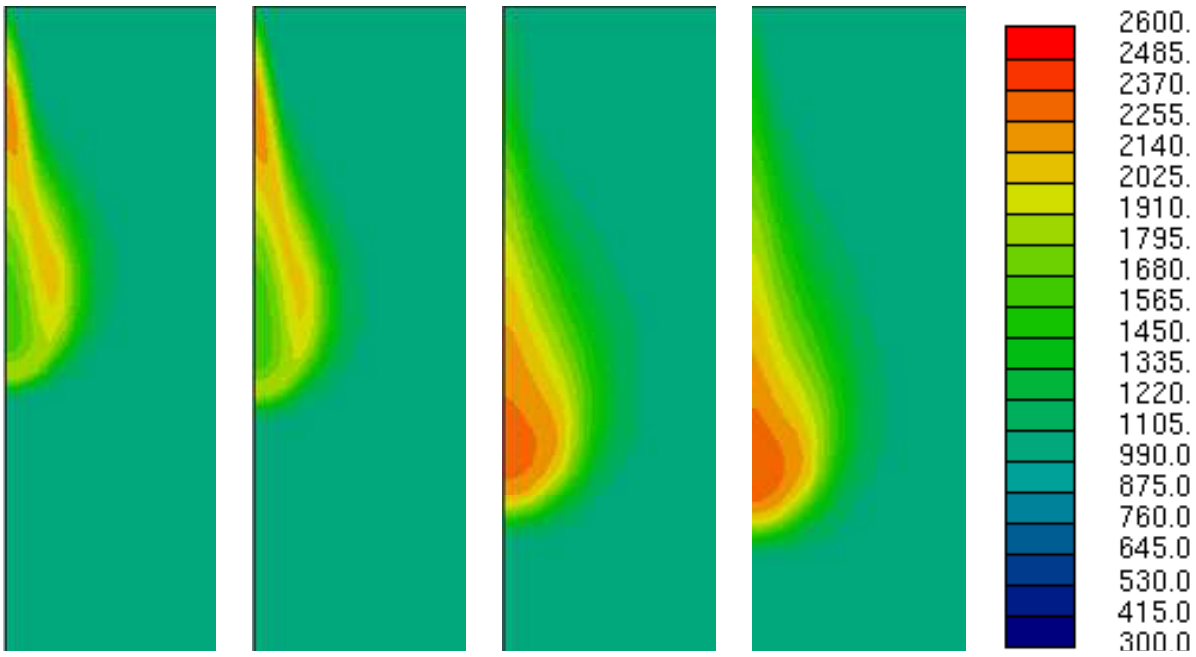

Figure 3. 2D profiles of temperature for the 20 % EGR case after 1 ms (a and b) and 2 ms (c and d). The unsteady flamelet library profiles (a and c) are virtually identical with the RIF (b and d) profiles. The temperature scale to the right is in Kelvin.

References

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