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Modeling of PCCI combustion with FGM tabulated chemistry

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HIGHLIGHTS

- FGM tabulated chemistry is applied to model PCCI combustion.
- Manifolds are generated with homogeneous reactor and counter-flow diffusion flamelet canonical systems.
- Auto-ignition delay characteristics of PCCI combustion is analyzed.

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ABSTRACT

Premixed Charge Compression Ignition (PCCI) is a new combustion concept aiming a simultaneous reduction of oxides of nitrogen and soot emissions. Therefore the operation focuses on improved fuel–air mixing before ignition and lower maximum in-cylinder temperatures during the complete engine cycle. In the PCCI-regime, the injection and ignition events do not overlap due to the longer ignition delay timings. As such ignition is not influenced by the injection event like in the conventional operation and it is essentially governed by chemical kinetics.

Numerical methods should incorporate flow and chemistry models in an accurate way. However, the computational demand for modeling these phenomena is high and the researchers work on several reduction techniques to achieve a practical computational efficiency. In this work the Flamelet Generated Manifold method is applied within the Computational Fluid Dynamics (CFD) framework to study PCCI combustion. In FGM, thermo-chemical properties are preprocessed by solving canonical systems (here, Igniting Counter-flow Diffusion Flamelets and Homogeneous Reactors) and stored in a manifold as a function of controlling variables.

Since ignition control is difficult in the aforementioned combustion concept, the accurate prediction of ignition phenomena is significant. Simulations are performed with three different mesh settings, where the course grid proves to be sufficiently accurate. Later the effect of multiple pressure levels is investigated using both canonical systems and the study shows that a number of three pressure levels is sufficient to capture the ignition phasing with Homogeneous Reactors based FGM tables. Finally, the sensitivity of ignition with respect to injection timing is shown to be predicted precisely.

1. Introduction

The conventional diesel operation (CI) leads to high levels of oxides of nitrogen (NO_x) and soot emissions. New combustion concepts target a simultaneous reduction of both emissions. Consequently new technologies emphasize obtaining a more homogeneous mixture and limiting local in-cylinder temperatures [1,2]. Homogeneous Charge Compression Ignition (HCCI), Premixed Charge Compression Ignition (PCCI), and Modulated Kinetics (MK) modify injection timings to enhance mixing prior to ignition. HCCI and PCCI combustion use early injection timings whereas MK applies late injection at or even after Top Dead Center (TDC) (see Fig. 1). Injecting the fuel in lower in-cylinder conditions prolongs ignition meaning more time for fuel-oxidizer mixing.

The main difference between the concepts of HCCI and PCCI is that the level of mixing is much higher for HCCI. Since the mixture in HCCI is almost homogeneous, the application is not feasible regarding the pressure rise rate limits at high loads.

In this work PCCI combustion [3–8] is studied. The operation of PCCI combustion decouples injection and heat release events. Since combustion starts after end of injection, the process is primarily governed by chemical kinetics and not by diffusive mixing anymore like in CI. A high amount of Exhaust Gas Recirculation (EGR) is also used to dilute the mixture and suppress in-cylinder temperature. As a result, concurrent reduction in NO_x and soot emissions can be attained. Since there is no more overlap between combustion and injection, no direct control over ignition is possible

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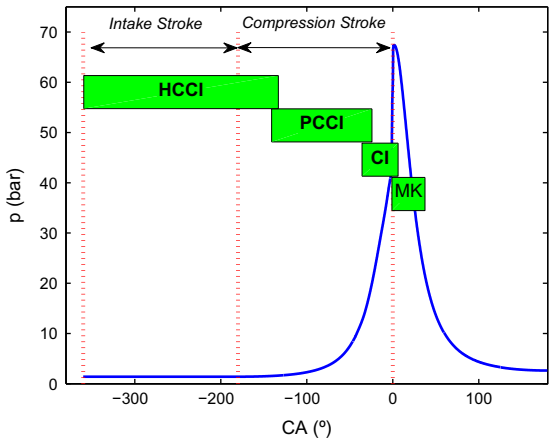

Fig. 1. Typical injection timings for different combustion systems. Blue line represents a typical pressure trace. Crank Angle (CA) = 0° stands for the TDC. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

which increases the significance of numerical modeling for PCCI combustion analysis.

A direct application of detailed reaction mechanisms within the CFD framework for complex systems like engines is not practical because of the number of additional equations and associated length and time scales. Therefore several reduction methods [9–14] exist for the reacting flows. Tabulated chemistry is used frequently to include detailed chemistry information in engine combustion modeling in a computationally efficient manner [15–22]. In this work, the Flamelet Generated Manifold (FGM) method is applied to model combustion. In the FGM approach, all thermo chemical properties are stored in a look-up table and characterized by the mixture fraction (Z) and a reaction progress variable ($\mathcal{Y}$). The method is initially based on the laminar flamelet concept [23], which assumes that a multi-dimensional flame is considered as a set of one dimensional (1D) flamelets. However, any appropriate canonical system can be applied during the FGM table generation. The approach has been applied successfully before in several applications [24–28]. Here it is implemented to analyze PCCI combustion.

In the next two sections theoretical background of the model and the experiment setup are described. In the results section, first the effects of different modeling parameters such as the mesh size and multiple pressure levels in FGM tabulation are investigated. Finally, a injection timing sweep is computed to assess the performance of the approach with respect to the ignition delay trend. The results are analyzed with respect to global parameters, being the pressure trace, ignition delay and heat release rate results.

2. Theoretical background

In the FGM tabulation, a chemistry database of relevant terms (a look-up table) is constructed and coupled to a Computational Fluid Dynamics (CFD) solver. In this way, the set of equations to be solved for chemistry is reduced to the number of controlling variables. Here, Z and $\mathcal{Y}$ are introduced to represent the evolution of mixing and chemistry, respectively. The definition of Bilger et al. [29] is introduced for Z,

$$Z = \frac{2\frac{Y_C - Y_{C,2}}{M_C} + 0.5\frac{Y_H - Y_{H,2}}{M_H} - \frac{(Y_O - Y_{O,2})}{M_O}}{2\frac{Y_{C,1} - Y_{C,2}}{M_C} + 0.5\frac{Y_{H,1} - Y_{H,2}}{M_H} - \frac{(Y_{O,1} - Y_{O,2})}{M_O}} \quad (1)$$

Above, Y and M are the mass fraction and molecular mass, respectively. Subscripts C, H, O refer to the carbon, hydrogen and oxygen elements and subscripts 1, 2 to the pure fuel and pure oxidizer concentrations, respectively.

The prerequisite for the $\mathcal{Y}$ definition is that it should be monotonic in time. Therefore a proper selection of species should be made. Here carbon monoxide (CO) and carbon dioxide (CO_2) are two major product species in any hydrocarbon combustion event. Hydroperoxyl (HO_2) is also included in the definition to increase the accuracy in the early phase of combustion.

$$\mathcal{Y} = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{HO_2}}{M_{HO_2}} \quad (2)$$

The first part of any FGM application is creating a representative manifold. For that relevant canonical systems need to be identified and compared. Two different methods are applied here, namely Igniting Counter-flow Diffusion Flamelets (ICDF) and Homogeneous Reactors (HR).

The first canonical system used in the FGM method is ICDF. The representative system is initiated by its success in the flamelet concept [23]. It is assumed that smallest time and length scales of the turbulent flow are larger than the chemical scales so that a thin and undisturbed chemical reaction zone exists and is not affected by the turbulent eddies.

Another canonical system that is used to generate the look-up table is HR. The main difference with the ICDF approach is that the absence of diffusion and transport processes (straining effect) in the evolution of the system. A perfect homogeneous fuel–air mixture is assumed and solved in time. To cover all possible mixing conditions a series of simulations (from pure fuel till pure oxidizer) are performed that correspond to the relevant range in mixture fraction space.

A coordinate free format is achieved by using controlling variables. Every thermo chemical property is stored as a function of these variables (Z and $\mathcal{Y}$). In the ICDF approach both igniting and stationary flames are solved at the corresponding initial conditions to cover the complete regime of diesel combustion. Igniting flames are solved at a single strain to capture the auto-ignition process. The ignition behavior is tracked until a steady state solution is obtained. The remaining area in $Z - \mathcal{Y}$ field is filled by solving a set of stationary flames at different strain rates (see Fig. 2a). In the HR approach there is no diffusion or any other transport phenomena, therefore the solutions are independent of each other. The solution starts (with $\mathcal{Y} = 0$) at each different mixture fraction point and evolves depending on chemical kinetics. Because of the combination of a low temperature and a very high equivalence ratio (φ), the mixture fails to ignite after a certain point in the mixture fraction space (see Fig. 2b).

Finally, the well-known presumed shape β-PDF approach is applied to include turbulence-chemistry interaction. The laminar table is integrated by applying the expected variances of the controlling variables in conjunction with the β-PDF's. Any mean quantity is then defined as follows,

$$\tilde{f} = \int_0^1 \int_0^1 f(Z,\mathcal{Y}) P(Z \| \tilde{Z}, \widetilde{Z''^2}) P(\mathcal{Y} \| \tilde{\mathcal{Y}}, \widetilde{\mathcal{Y}''^2}) dZ d\mathcal{Y} \quad (3)$$

The second part of the FGM application is the implementation of the manifold in the CFD code (here, STAR-CD).

The FGM table is used as a look-up table during the CFD computation. For that one extra transport equation is solved in the CFD code for each controlling variable and depending on the approach taken one extra for its variance. Relevant terms are retrieved from the manifold depending on these controlling variables and their variances. The Lagrangian spray model for liquid injection is solved in the CFD model and the evaporation of fuel acts as a source term in Z. The coupling between FGM-CFD is completed by returning the values for the source term of progress variable ($\dot{\mathcal{Y}}$) and species