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Probability density function approach coupled with detailed chemical kinetics for the prediction of knock in turbocharged direct injection spark ignition engines

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ABSTRACT

In this work a new knock model is derived which accounts for the inherent feature of knocking combustion, namely that it is a stochastic phenomenon. It provides the probability of autoignition and distinct criteria to determine the mean knock onset as well as the relative number of knocking cycles. For modeling purposes an ignition progress variable is proposed to determine the reactive state of the unburnt fuel–air mixture and the occurrence of autoignition. Statistical information of this quantity is introduced by presuming a clipped Gaussian probability density function (PDF). Its shape is defined by the Favre mean and variance of the ignition progress variable for which transport equations are derived. The chemical source terms that appear in these equations are closed by employing a presumed PDF approach to account for turbulence chemistry interaction. A clipped Gaussian PDF distribution for temperature and a β-PDF for mixture fraction are employed. Hence, the impact of temperature and mixture fraction fluctuations on the ignition progress variable is accounted for. The chemical source terms are evaluated based on tabulated chemistry incorporating detailed chemical kinetics. For the assessment of the knock model a spark timing sweep was performed on the engine test bench for a full-load operating point at $n = 2000$ rpm. In-cylinder flow simulations including gas exchange, mixture formation, combustion, and knock were carried out and the results are compared with experimental data. It is shown that the knock model is able to predict the mean knock onset with reasonable accuracy and that the impact of a spark timing sweep on the number of knocking cycles is well captured.

1. Introduction

Extensive experimental and numerical investigations have been carried out since the beginning of the 20th century to explain the origin and the consequences of knocking combustion. It is characterized by a high peak pressure and pressure oscillations in the combustion chamber and can lead to severe damage or complete destruction of the engine. There exist various ways to initiate knocking combustion in spark ignition (SI) engines: the ignition of the unburnt fuel–air mixture by hot spots on combustion chamber walls, glowing carbon particles, autoignition processes, or by ignitable droplets of lubricant oil. If the combustion starts before the spark timing, it is referred to as pre-ignition. An overview of the different types of knocking combustion and its causes is given by Dahnz and Spicher [1], where special emphasis is put on an analysis of irregular combustion phenomena in supercharged SI engines caused by pre-ignition. The severity of the knocking event depends on the propagation mode of the reaction wave induced by an exothermic center. Depending on the local instantaneous temperature gradient it is possible that a detonation wave is initiated, which is responsible for the aforementioned high peak pressure and pressure oscillations in the combustion chamber. An investigation and discussion of the various modes of reacting front propagation is given by Zeldovich [2], Gu et al. [3], and Bradley et al. [4].

This work focuses on engine knock that is initiated by autoignition of the unburnt fuel–air mixture ahead of the flame front. It is a fundamental issue of SI engines. The autoignition process is triggered by compression of the unburnt fuel–air mixture. This compression is caused by the pressure rise of both the moving piston and the expanding flame front. Autoignition can be controlled by adjusting the spark timing: advancing the spark timing increases the knock intensity and vice versa. Hence, this type of knocking combustion is often referred to as spark knock [5]. Due to the retarded spark timing, the propagation of the flame front and the compression of the unburnt mixture is shifted into the expanding exhaust stroke, and hence critical thermodynamic states are

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avoided. This leads inevitably to a decrease in thermal efficiency and poor engine performance, since the combustion process does not occur at the optimum timing within the engine cycle. Due to the increasing demand for both maximum engine output and minimum fuel consumption, the engine has to be operated close to the allowable knock limit. Hence, knocking combustion is a crucial constraint in the engine development process. The derivation of countermeasures against knock has become even more important for modern turbocharged direct injection spark ignition (DISI) engines, which are operated under higher specific loads compared to naturally aspirated engines.

1.1. Current modeling approaches

A major difficulty in modeling knock lies in its erratic nature, the cycle-by-cycle variations as well as in a clear and distinct description of the knocking event. Even the experimental evaluation and characterization is not straightforward and an in-depth experience and expertise is needed. By modeling knocking combustion it is commonly assumed that knock is caused by autoignition of a pocket of fuel–air mixture ahead of the flame front. Hence, most of the existing three-dimensional knock models aim to describe the autoignition process in the unburnt mixture. The employed modeling strategies can be roughly subdivided into two different approaches: a direct modeling of the autoignition process and models based on a pseudo precursor that determines the reactive state of the unburnt fuel–air mixture.

In order to determine the autoignition process, it is necessary to incorporate detailed chemical kinetics. Due to the high computational costs, detailed chemical reaction mechanisms are often avoided and simple approaches like the Shell autoignition model [6–10] are employed. Eckert et al. [11] have simulated knock in SI engines by means of a 3D-CFD approach. The autoignition chemistry was computed using a reduced chemical reaction mechanism based on the Shell model. The presented approach is solely based on mean quantities and turbulence chemistry interaction is not accounted for. An autoignition model based on tabulated chemistry and a presumed temperature PDF has been proposed by Truffin and Colin [12]. The model was applied to compute the combustion in a Homogeneous Charge Compression Ignition (HCCI) engine. It was shown that it is of significant importance to account for the impact of temperature fluctuations on the autoignition process. Knop et al. [13] have used the tabulation approach to model autoignition in SI engine. Here, the autoignition process was computed based on the tabulation of ignition delay times and reaction rates, whereas the flame propagation was modeled with a coherent flame model (CFM). Moreover, a new coupling approach based on an additional progress variable accounting for the fuel consumption by the autoignition process was presented. The validation of the model was performed based on a naturally aspirated and a turbocharged operating point, showing reasonable agreement between simulation results and experimental data.

Models based on a pseudo precursor assume that the chemical state of a reacting mixture can be represented by the concentration ratio $[x]/[x_c]$ of a significant species. The critical concentration $[x_c]$ corresponds to the species concentration at time of ignition. Livengood and Wu [14] proposed that there is a functional relationship between the rate of change of the concentration ratio and the inverse of the ignition delay time τ of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{[x]}{[x_c]}\right)=\frac{1}{\tau}. \tag{1}$$

The temporal integration from the time where no appreciable reaction has begun to the time t_k when knock or autoignition occurs leads to

$$\left(\frac{[x]}{[x_c]}\right)_{t_k}=\int_{t=0}^{t_k}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{[x]}{[x_c]}\right)\mathrm{d}t=\int_{t=0}^{t_k}\frac{1}{\tau}\,\mathrm{d}t=1. \tag{2}$$

This equation is commonly referred to as the Livengood-Wu integral. Lafossas et al. [15], and Teraji et al. [16] have introduced a pseudo precursor to define the onset of autoignition in a 3D-CFD simulation. Both models perform the integration of the pseudo precursor locally. No transport equation is solved. Moreover, statistical information regarding the probability of autoignition was not provided and the effect of turbulence chemistry interaction was neglected.

Despite the recent successful applications of multi-cycle Large Eddy Simulations (LES) of IC engines targeting combustion induced cycle to cycle variations (CCV) [17–19], the 3D-CFD codes used in industrial applications are based on the Reynolds-averaged Navier–Stokes (RANS) equations. RANS-based models are extensively used because of their computational efficiency. However, cyclic variations are not considered in this approach and the interpretation of the CFD results with respect to knock onset, knock intensity, and number of knocking cycles is rather difficult. The effect of cyclic variations on these criteria is illustrated in Fig. 1, where measured pressure traces for 1000 consecutive cycles for a full-load engine operating point at 5000 rpm are shown. Additionally, the corresponding averaged pressure trace is depicted and is represented by the solid black line. The cycle-by-cycle variations are clearly visible. These variations lead to different peak pressures, changes in heat release rate, and to irregular combustion phenomena. From these 1000 consecutive cycles 270 were identified as knocking cycles. A simulation of this engine operating point with a RANS CFD code yields a pressure trace very similar to the solid black line in Fig. 1. It is obvious that an evaluation of knock criteria solely based on averaged quantities is quite limited. More strictly speaking, it is not possible to deduce the impact of knocking combustion for the investigated engine operating point from the mean pressure history in Fig. 1. Hence, for a sound prediction of knocking combustion it is of significant importance to provide statistical information regarding the formation of engine knock. From the discussion given above it may appear that an LES-based model is the most suitable approach to simulate knock in IC engines, since the cyclic variations are directly resolved. However, the use of an LES

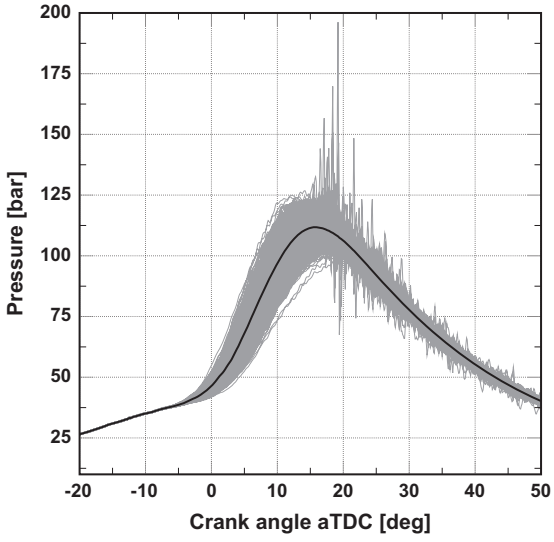

Fig. 1. Measured pressure traces for 1000 consecutive cycles where 270 were identified as knocking cycles. The measurements were taken for a full-load engine operating point at 5000 rpm. The solid black line represents the averaged pressure history.