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Scalar dissipation rate based multi-zone model for early-injected and conventional diesel engine combustion

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ABSTRACT

Low-temperature combustion (LTC) concepts, such as Homogeneous Charge Compression Ignition (HCCI) or Premixed-Charge Compression Ignition (PCCI), have the potential of simultaneous reducing nitrogen oxides (NO_x), soot, and unburned hydrocarbons (uHC). However, the successful implementation for internal combustion engines is difficult. Control strategies need to be employed to ensure appropriate combustion phasing over wide ranges of operating conditions. Model-based engine control is particularly successful when physics-based models are employed. Multi-zone combustion models represent potential candidates for efficiently computing combustion in PCCI diesel engines. Multi-zone models were originally developed for HCCI gasoline engine combustion and did not account for mixing between zones due to the relatively homogeneous mixture while later developments considered small inhomogeneities. However, for diesel or PCCI combustion, this is not justified due to noticeable fuel stratification. Therefore, a novel mixing model for multi-zone modeling accounting for mass and energy exchange between zones is presented in this work. The model is derived from the representative interactive flamelet (RIF) model and thus depends on the scalar dissipation rate as well as the mixture fraction in each zone. The multi-zone model can be used as a stand-alone model after performing a number of non-reactive computational fluid dynamics (CFD) simulations to train an empirical, engine-specific model for the scalar dissipation rate. With the stand-alone model, cost-efficient parameter studies can be performed, with further model reduction, the use in model-based control algorithms is also possible. For validation of the stand-alone multi-zone model, experiments were conducted with a four-cylinder diesel engine. 105 operation conditions including variations in start of injection (SOI), injected fuel mass (FMI), and external exhaust gas recirculation (EGR) were selected to assess the model performance. CFD simulations applying the RIF model were carried out for representative cases to further assist in validating and analyzing the new multi-zone model. Predictions of the multi-zone model regarding indicated mean effective pressure (IMEP), combustion phasing (CA_{50}), and emissions of nitrogen monoxide as well as unburned hydrocarbons are compared against experimental data and results from numerical simulations. Overall good agreement over various operating conditions was found demonstrating the capability of the multi-zone model to adequately capture PCCI diesel engine combustion.

1. Introduction

In search of new combustion concepts that are less polluting while at the same time more fuel efficient, low-temperature combustion (LTC) was proposed. For diesel engines, Premixed Charge Compression Ignition (PCCI), which is the focus of the present paper, has emerged as an interesting alternative to conventional diesel combustion in the part-load operating range [1–3]. It involves relatively early injection timings, thus providing more time for fuel–air mixing. This results in less diffusion-controlled combustion and hence reduced soot emissions. Improved homogenization also reduces peak in-cylinder temperatures and facilitates reduced nitrogen oxide (NO_x) emissions when combined with high external exhaust gas recirculation (EGR) rates. A general review of LTC concepts may be found in [4,5].

However, one of the major challenges for early direct-injection PCCI combustion is the tendency for combustion to occur mainly before top dead center (TDC), which often increases noise and reduces engine efficiency. Sophisticated model-based closed-loop control of the combustion process is one means to overcome this difficulty. To improve current controller models [6–9], more physical and chemical insight needs to be incorporated. This requires

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the development of efficient but accurate physics-based combustion models, which is challenging due to the strong nonlinearities of the physical and chemical processes encountered in PCCI diesel engine combustion.

In that regard, multi-zone combustion models have gained substantial consideration in recent years from both academia and industry. Originally developed for HCCI combustion, multi-zone modeling frameworks were formulated without considering mixing between the individual zones [10–12]. To incorporate mixing effects, these approaches were modified by interactively coupling computational fluid dynamics (CFD) and multi-zone codes [13–15]. However, mixing in phase space is based on the turbulent time scales resolved by the flow solver and neither considers micro-scale mixing nor the relevant chemical scales. As a consequence, these frameworks may not be fully suitable to capture effects of turbulence-chemistry interactions in processes such as ignition or extinction where substantial relative progress of heat release and chemical kinetics occurs over turbulent time scales.

In an effort to address this shortcoming, Barths et al. [16] developed a mixing model for the two-way coupling of CFD codes with a multi-zone model. Upon initialization of the multi-zone model, all CFD cells are ordered based on the mixture fraction variable and are subsequently binned into several chemistry zones. Then, two streams of information are interactively exchanged at every CFD time step. In the CFD code, the change of the mixture fraction distribution is evaluated and passed to the multi-zone model in the form of a mixing rate. Vice versa, the heat release is calculated in each chemistry zone and passed to its associated CFD cells. This approach was also applied to PCCI diesel engine combustion and validated against experimental data [17,18]. Additionally, a stand-alone multi-zone model was systematically derived from the coupled 3D CFD approach that is aimed for use in model-based control [17]. However, the chosen mixing approach lacks physical meaning and fails to predict PCCI combustion for varying injected fuel mass and exhaust gas recirculation. Therefore, a novel mixing model is presented in this work that is derived from the Representative Interactive Flamelet (RIF) model. Mixing between zones is then determined by the scalar dissipation rate and the mixture fraction in each zone.

Results with the stand-alone multi-zone model are compared to data from CFD simulations fully coupled with the RIF model, referred to as CFD RIF, and with engine experiments. In-cylinder pressure data and engine-out emissions are considered. The experimental data comprise 105 different operating conditions with start of injection varying between 45.4° and 5.4° bTDC, injected fuel mass between 8.5 and 17.5 mm^3 per cycle and external exhaust gas recirculation from 0% to 50%. In this way, the prediction capability of the novel multi-zone model can be assessed over wide ranges of operating conditions.

This paper is arranged as follows: Section 2 deals with the combustion modeling approach employed in the present investigation. Theory and assumptions underlying the multi-zone model and the derivation of the inter-zonal mixing model are presented and discussed. Section 3 describes the experimental and numerical setups. Finally, in Section 4, results of the multi-zone model are compared to CFD RIF and experimental data.

2. Computational models

In this section, the applied computational models are introduced and the governing equations presented. First, the CFD RIF model is discussed. Then, an outline of the multi-zone model is given and the mixing model is derived. Different approaches to determine the scalar dissipation rate appearing as a parameter in the mixing model are illustrated. Finally, the chemistry model is presented.

2.1. CFD RIF model

3D CFD simulations were performed with the flow solver AC-FluX applying the representative interactive flamelet (RIF) model. The flamelet model can be rigorously derived from the governing equations [19] under the assumption that combustion is relatively fast compared with the small scale turbulent motions, and the RIF model has been derived particularly for describing unsteady ignition and combustion processes in compression ignition engines [20,21]. This model has been successfully applied for diesel engine simulations [22–25] and recently has been tested and validated using DNS data [26,27]. Flamelet modeling has the advantage of separating the numerical effort associated with the resolution of small time and length scales arising from the interaction of small-scale mixing with chemistry from the numerical effort of the CFD computation of the engine combustion cycle.

The basis for deriving the flamelet equations is the mixture fraction Z, which is a measure for the local equivalence ratio in the flow field. The mixture fraction is a scalar which can be defined by the transport equation

$$\rho\frac{\partial Z}{\partial t}+\rho v_\alpha\frac{\partial Z}{\partial x_\alpha}-\frac{\partial}{\partial x_\alpha}\left(\rho D_Z\frac{\partial Z}{\partial x_\alpha}\right)=\dot{\rho}_{\mathrm{inj}} \tag{1}$$

with the boundary conditions $Z=1$ for pure fuel and $Z=0$ for pure oxidizer [28]. The diffusion coefficient D_Z is chosen such that the Lewis number Le_Z is equal to unity and $\dot{\rho}_{\mathrm{inj}}$ accounts for the source term due to fuel injection, which is determined by the spray model.

The unsteady flamelet equations have been derived by Peters [19,29] and can be written as

$$\frac{\partial T}{\partial t}=\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2}+\frac{\chi}{2c_p}\left(\sum_j^{n_s}c_{pj}\frac{\partial Y_j}{\partial Z}+\frac{\partial c_p}{\partial Z}\right)\frac{\partial T}{\partial Z}-\frac{1}{\rho c_p}\left(\sum_j^{n_s}h_j\dot{m}_j-\frac{\partial p}{\partial t}-S_{\mathrm{inj}}\right) \tag{2}$$

and

$$\frac{\partial Y_j}{\partial t}=\frac{\chi}{2}\frac{\partial^2 Y_j}{\partial Z^2}+\frac{\dot{m}_j}{\rho}+\frac{\dot{\rho}_{j,\mathrm{inj}}}{\rho}. \tag{3}$$

In these equations, n_s denotes the number of chemical species, p is the pressure, c_{pj}, $\dot{m}_j$, h_j, and Y_j are the specific heats at constant pressure, the chemical production rates, the enthalpies, and the mass fractions of the chemical species j, respectively. The influence of fuel vaporization on species mass fractions and enthalpy is represented by the source terms $\dot{\rho}_{j,\mathrm{inj}}=\dot{\rho}_{\mathrm{inj}}(\delta_{lj}-Y_j)$ and $S_{\mathrm{inj}}=\dot{\rho}_{\mathrm{inj}}(h_{\mathrm{inj}}-\sum_j Y_j h_j)$, respectively, which represent the evaporated fuel mass and energy per unit volume and time. Here, δ is the Kronecker symbol, l denotes the evaporating liquid component, and h_{inj} is the enthalpy of the evaporated fuel evaluated at injection conditions and taking into account the latent heat of vaporization. In analogy to the multi-zone model, fuel is only added to the fuel side ($Z=1$). Therefore, the drift terms due to evaporation vanish. A derivation of the flamelet equations with convective terms due to spray evaporation may be found in [30]. Both source terms, $\dot{\rho}_{j,\mathrm{inj}}$ and S_{inj}, are calculated in the CFD code and provided to the RIF model.

In Eqs. (2) and (3), no convective terms appear. This is due to the fact that all scalars such as Z, T, and Y_j are transported with the same convection velocity. In both equations however, the first term on the right hand side contains the scalar dissipation rate, introduced as

$$\chi=2D_Z\left(\frac{\partial Z}{\partial x_\alpha}\right)^2, \tag{4}$$

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