

Applying an Interactively Coupled CFD-Multi-Zone Approach to Study the Effects of Piston Bowl Geometry Variations on PCCI Combustion

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ABSTRACT

Recently, a consistent mixing model for the two-way coupling of a CFD code and a zero-dimensional multi-zone code was developed. This work allowed for building an interactively coupled CFD-multi-zone approach that can be used to model HCCI combustion.

In this study, the interactively coupled CFD-multi-zone approach is applied to PCCI combustion in a 1.9l FIAT GM Diesel engine. The physical domain in the CFD code is subdivided into multiple zones based on one phase variable (fuel mixture fraction). The fuel mixture fraction is the dominant quantity for the description of nonpremixed combustion. Each zone in the CFD code is represented by a corresponding zone in the zero-dimensional multi-zone code. The zero-dimensional multi-zone code solves the chemistry for each zone, and the heat release is fed back into the CFD code. The thermodynamic state of each zone, and thereby the phase variable, changes in time due to mixing and source terms (e.g., vaporization of fuel, wall heat transfer). An elaborated mixing model and an appropriate treatment of the source terms keep the thermodynamic state of the zones in the CFD code and the zero-dimensional multi-zone code identical.

The results obtained with the interactively coupled CFD-multi-zone approach are compared to experimental results for five selected operating conditions, showing very good agreement. In a following step, the engine geometry used in the numerical simulations is modified, yielding two different piston-bowl geometries which vary from the original shape in regard to bowl diameter and bowl depth. The volume of the bowl and thus the compression ratio are kept at the original value. Simulations of PCCI combustion using these modified geometries show the influence of the piston-bowl shape on mixture formation and pollutant emissions, leading the way to numerically optimise the piston-bowl design for PCCI combustion.

INTRODUCTION

There is a strong demand to explore new combustion concepts capable of meeting future emission standards, such as Tier 2 Bin 5 on the North American market or EURO V on the European market. Premixed Charge Compression Ignition (PCCI), or Premixed Compression Ignition (PCI), as it is sometimes referred to, has emerged as an interesting alternative to conventional Diesel combustion in the part-load operating range [15, 20, 29]. This concept involves relatively early injection

timings, high external EGR rates, and cooled intake air, leading to a low-temperature combustion (LTC) process with low NO_x and particulate emissions. A general review of LTC processes can be found in [7]. However, in contrast to conventional Diesel combustion, with early direct-injection LTC it can be difficult to prevent combustion from occurring before top dead center (TDC), which often increases noise and reduces engine efficiency.

Many combustion modelling approaches, such as the Representative Interactive Flamelet (RIF) concept [6, 9, 16, 26] were extensively tested and validated in the limit of highly stratified fuel-air mixtures. In the limit of nearly homogeneous fuel-air mixtures, multi-zone models proved successful [1, 2, 4]. However, in order for CFD modelling to play a role in providing guidelines in the development of new PCCI combustion concepts, the applicability of all these modelling approaches to the PCCI combustion regime still has to be tested thoroughly.

Correctly capturing the physics and chemistry underlying partially premixed compression ignition in Diesel engines poses a tremendous modelling challenge. Whereas all combustion modelling relies on adequate descriptions of fluid dynamics, liquid-phase, and chemistry, capturing the phenomena pertaining to partially premixed Diesel combustion stretches the limits in each of these areas. Ignition timing is governed both by turbulent mixing and chemistry. Since Diesel fuel displays significant low-temperature chemistry in the thermodynamic ranges relevant for engine operation, it is necessary that the reaction mechanism used to model heat release is capable of capturing this. Furthermore, the very advanced injection timings required to yield a sufficiently homogeneous mixture at the time of ignition are likely to lead to substantial wall impingement. The latter is a rather complex process to model.

This paper is arranged as follows: The first section deals with the combustion modelling approach employed in the current investigation. The coupling of the three-dimensional CFD code to the multi-zone chemistry model is shortly described. After this, the four-cylinder test engine, the investigated operating points, as well as the corresponding numerical setup and the modifications to the piston-bowl geometry, are presented. The next section contains the validation of the numerical simulations against the experiment, using the original piston-bowl geometry. Following this, simulations using modified bowl geometries are presented, showing the influence of piston-bowl design on mixture formation and combustion. Finally, the conclusions and major findings from the study are summarized. Frequently used definitions, acronyms, and abbreviations are included at the end of the paper, following the references.

COMBUSTION MODEL FORMULATION

MULTI-ZONE CHEMISTRY MODEL

Multi-Zone Modeling Overview In HCCI or PCCI engines, where substantial premixing occurs, the cylinder charge may be divided into several distinct regions, each characterized by a certain thermodynamic state. A major requirement is for the variance within each individual zone to be small, since the multi-zone chemistry code solves only for the average values provided.

Several multi-zone approaches have been proposed in the literature. Aceves et al. [1, 2] used zones based on the temperature to account for thermal gradients inside the cylinder of heavy-duty truck engines running in HCCI mode on natural gas and propane.

Babajimopoulos et al. [4] used equivalence ratio, temperature, and EGR to define the zones in investigating various variable valve actuation (VVA) strategies in a heavy-duty truck engine fueled by natural gas. In all these studies, the zones were initialized based on three-dimensional CFD calculations of the flow up to a certain crank angle at which chemical reactions start to occur. The mass of each zone was primarily governed by the given temperature distribution in the cylinder, and no mixing occurred between the zones in the multi-zone chemistry code. In the study by Babajimopoulos et al. [4], each temperature zone was divided into three equivalence ratio zones of equal mass.

In a more recent publication, Babajimopoulos et al. [3] extended the sequential approach presented in [4] to a fully coupled computational fluid dynamics and multi-zone model with detailed chemical kinetics. The multi-zone model communicated with the CFD code at each computational time step, and the composition of the CFD cells was mapped back and forth between the CFD code and the multi-zone model. This approach was validated against experimental data in [13] and [18].

Multi-Zone Model The multi-zone model employed in the current study is X0D, a zero-dimensional chemistry solver based on multiple zero-dimensional reactors. X0D was developed internally at General Motors R&D by Hardo Barths, Tom Sloane, and Christian Hasse, and was first described in Hergart et al. [17] and Felsch et al. [11].

The equations governing species mass fractions, temperature, and pressure change in the multi-zone chemistry code are given below:

$$\frac{dY_{ij}}{dt} - \frac{1}{m_i} \sum_{k=1}^{nz} \dot{m}_{ik} (Y_{kj} - Y_{ij}) - \frac{\dot{\omega}_{ij}}{\rho_i} - \frac{\dot{\rho}_{ij}^s}{\rho_i} = 0, \quad (1)$$

$$\begin{aligned} \frac{dT_i}{dt} - \frac{1}{m_i \cdot \bar{c}_{pi}} \sum_{k=1}^{nz} \dot{m}_{ik} (\bar{h}_k - \bar{h}_i) \\ + \frac{1}{m_i \cdot \bar{c}_{pi}} \sum_{j=1}^{nsp} h_{ij} \sum_{k=1}^{nz} \dot{m}_{ik} (Y_{kj} - Y_{ij}) \\ + \frac{1}{\rho_i \cdot \bar{c}_{pi}} \sum_{j=1}^{nsp} h_{ij} \cdot \dot{\omega}_{ij} - \frac{1}{\rho_i \cdot \bar{c}_{pi}} \frac{dp}{dt} \\ - \frac{1}{\rho_i \cdot \bar{c}_{pi}} \sum_{j=1}^{nsp} \dot{\rho}_{ij}^s \cdot \Delta h_{vj} + \frac{1}{m_i \cdot \bar{c}_{pi}} \dot{Q}_{wall,i} = 0, \quad (2) \end{aligned}$$

and

$$\begin{aligned} \frac{dp}{dt} = - \frac{p}{V} \frac{dV}{dt} \\ + \frac{p}{V} \sum_{i=1}^{nz} V_i \left(\frac{1}{m_i} \frac{dm_i}{dt} + \frac{1}{T_i} \frac{dT_i}{dt} + \bar{M}_i \sum_{j=1}^{nsp} \frac{1}{M_j} \frac{dY_{ij}}{dt} \right). \quad (3) \end{aligned}$$

In Eq. (1), Y_{ij} denotes the mass fraction of species j in zone i , Y_{ik} denotes the mass fraction of species j in neighbouring zone k , and $\dot{\omega}_{ij}$ is the corresponding chemical source term in zone i . $\dot{\rho}_{ij}^s$ accounts for the source term due to fuel vaporization. It is zero for all species except the fuel itself ($\dot{\rho}_{ij}^s = 0, j \neq \text{fuel}$). The second term on the left-hand side of Eq. (1) describes the species exchange between the zones, where $\dot{m}_{ik}$ is the rate at which species mass fractions are transported between zone i and neighbouring zone k . Thereby, nz stands for the total number of zones. Similarly, in Eq. (2) the second and third term on the left-hand side represent the enthalpy exchange between zones due to enthalpy stratification between zones and due to species stratification between zones, respectively. $\bar{h}_k$ and $\bar{h}_i$ denote the average specific enthalpies for zones k and i . Δh_{vj} denotes the latent heat of vaporization of species j , and $\dot{Q}_{wall,i}$ is the wall heat transfer of zone i . In Eqs. (2) and (3), nsp accounts for the number of species employed in the underlying chemical mechanism. The equation of state is used to derive Eq. (3), which solves for the pressure across the zones. Through this equation, all zones are thermodynamically coupled with each other.

Wall heat transfer is described as

$$\dot{Q}_{wall,i} = \sum_{l=1}^{n_{wall}} A_{wall,l,i} \cdot h_{wall,l,i} (T_i - T_{wall,l}), \quad (4)$$

where n_{wall} denotes the total number of walls in the engine, $A_{wall,l,i}$ the area of wall l belonging to zone i , $h_{wall,l,i}$ the heat transfer coefficient of zone i to wall l , T_i

the temperature of zone i , and $T_{wall,l}$ the temperature of wall l .

The mixing in the multi-zone model is accounted for by allowing the different zones to exchange species composition and enthalpy with each other, in addition to the interaction through the pressure. The mass of each zone is kept constant and the model can accommodate any number of zones.

Chemistry Model A major aspect in modelling Diesel engine combustion is the treatment of the chemistry. Combustion chemistry in X0D is described by a detailed chemical mechanism that comprises 59 elementary reactions among 38 chemical species. This mechanism describes low-temperature auto-ignition and combustion of n-heptane, which serves as a surrogate fuel for Diesel in this work. In addition, it accounts for thermal NO formation. The chemical mechanism for n-heptane was constructed by Peters et al. [25]. The NO-submechanism, which is part of the full mechanism, is the extended Zeldovich mechanism [19].

CFD CODE The CFD code used in this work is AC-FluX (formerly known as GMTEC), a flow solver based on Finite Volume methods [12] that employs unstructured, mostly hexahedral meshes. AC-FluX solves for the partial differential equations for continuity, the Navier-Stokes equations, an equation for the total enthalpy, and two equations to account for the turbulence (k-epsilon-model). AC-FluX is documented by Khalighi et al. [21] and by Ewald et al. [8].

The liquid phase is modeled using the discrete droplet model (DDM), which approximates the spray by a Monte-Carlo simulation. Since the spray consists of a large number of droplets, only the behaviour of a representative subset of all droplets (called parcels) is calculated in detail. The gas phase and the liquid phase are coupled through source terms in the governing equations for the gas phase. A detailed description of the spray modelling in AC-FluX can be found in Spiekermann et al. [28]. The spray model parameters are always subject to adjustment and were adapted such that the pressure curve for TS-3 matched the experimental results (see Sec. "Operating Conditions" for details on TS-3). The parameters used in this work are within the recommended parameter range proposed by Weber et al. [32].

The composition of the charge is represented by four so-called active species streams, which are the mass fraction of fuel $\tilde{Y}_{fuel}$, the mass fraction of air $\tilde{Y}_{air}$, the mass fraction of combustion products (carbon dioxide and water) $\tilde{Y}_{products}$, and the mass fraction of residuals $\tilde{Y}_{EGR}$. The corresponding transport equation reads

$$\frac{\partial \bar{\rho} \tilde{Y}_j}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_i \tilde{Y}_j}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho} D_j \frac{\partial \tilde{Y}_j}{\partial x_i} \right) + \bar{\rho} \dot{\omega}_j + \dot{\rho}_j^s. \quad (5)$$

In Eq. (5), $\tilde{Y}_j$ denotes active species stream j , $\bar{\rho}$ the density, $\tilde{v}$ the velocity, D_j the diffusion coefficient of active stream j , and $\dot{\omega}_j$ the chemical source term of active stream j . The source term for the residuals is identical zero ($\dot{\omega}_{\text{EGR}} = 0$), because they are assumed to be chemically inert. The residuals are therefore an indicator for dilution in the CFD code. The term $\dot{\rho}_j^s$ represents the source term due to fuel vaporization. It is zero for all species except the fuel itself ($\dot{\rho}_j^s = 0, j \neq \text{fuel}$).

For the interactive coupling to the multi-zone model X0D, two additional scalars are introduced. These are the fuel mixture fraction Z_{fuel} and an artificial scalar S .

The fuel mixture fraction Z_{fuel} is the dominant quantity for the description of nonpremixed combustion and can be related to the commonly used equivalence ratio ϕ according to

$$\phi = \frac{Z_{\text{fuel}}}{1 - Z_{\text{fuel}}} \frac{(1 - Z_{\text{fuel,st}})}{Z_{\text{fuel,st}}}, \quad (6)$$

where $Z_{\text{fuel,st}}$ is the fuel mixture fraction at stoichiometric mixture [24]. In the CFD code, a transport equation for the mean fuel mixture fraction $\tilde{Z}_{\text{fuel}}$ is solved, reading

$$\frac{\partial \bar{\rho} \tilde{Z}_{\text{fuel}}}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_i \tilde{Z}_{\text{fuel}}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho} D_Z \frac{\partial \tilde{Z}_{\text{fuel}}}{\partial x_i} \right) + \dot{\rho}_{\text{fuel}}^s. \quad (7)$$

Similar to Eq. (5), the term $\dot{\rho}_{\text{fuel}}^s$ represents the source term due to fuel evaporation.

In addition to the transport equation for the mean fuel mixture fraction $\tilde{Z}_{\text{fuel}}$, a generic convection diffusion equation without source terms is considered for the mean artificial scalar $\tilde{S}$. This transport equation reads

$$\frac{\partial \bar{\rho} \tilde{S}}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_i \tilde{S}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho} D_S \frac{\partial \tilde{S}}{\partial x_i} \right). \quad (8)$$

It is assumed that the diffusion coefficients D_j , D_Z , and D_S are identical.

Solving Eqs. (7) and (8) is mandatory in order to establish the interactive coupling of the CFD code AC-FluX and the multi-zone model X0D. The interactive coupling is described in the following section.

INTERACTIVE COUPLING OF CFD CODE AND MULTI-ZONE MODEL The two-way-coupling (interactive coupling) of CFD codes and zero-dimensional multi-zone codes was introduced by Barths et al. [5]. It is also described in detail by Felsch et al. [10]. In this section, the main aspects regarding the interactive coupling of the CFD code AC-FluX and the multi-zone model X0D are discussed. After initialization, the interactive coupling comprises one information stream which is fed from the CFD code to the multi-zone model. Mixing effects are introduced into the multi-zone model based on the CFD solution. Vice versa, one information stream is fed from the multi-zone model to the CFD code in order to keep the heat release consistent between both codes. These issues are addressed in Secs. “Initialization of the Interactive Coupling”, “Mixing Model”, and “Consistency of Heat Release”. Section “Treatment of Source Terms” deals with the treatment of source terms within the interactive coupling.

Initialization of the Interactive Coupling In order to construct the mass distribution function and subdivide it into discrete zones in phase space, the computational cells in the physical CFD domain are sorted in ascending order in terms of the mean fuel mixture fraction $\tilde{Z}_{\text{fuel}}$. The computational cells are then assigned to the zones so that these have equal mass. This is not a requirement, but it simplifies the derivation and implementation. This procedure is repeated at each time step of the CFD code. Only once, however, at a certain crank angle prior to any chemical reactions starting to occur, a corresponding set of zones defined by a specific fuel mass, temperature, and residual mass fraction is initialized in the multi-zone model X0D. In addition, at this transition point the distribution of the mean mixture fraction $\tilde{Z}_{\text{fuel}}$ is mapped on the mean artificial scalar $\tilde{S}$. After initialization of the multi-zone model, both codes interact back and forth throughout the engine cycle. The two codes run independently but simultaneously, without any reinitialization of the zones (and the numerical solver for the differential equations) in the multi-zone model.

Fig. 1 schematically illustrates how the AC-FluX CFD code is used to initialize the zones in X0D, for which the chemistry is solved. For the reference case TS-3 (see Secs. “Experimental Setup” and “Numerical Setup” below), the left-hand side of Fig. 1 shows the injector cut plane coloured by zone affiliation at time of X0D initialization. The zone affiliation is the result of the sorting procedure outlined above. Upon initialization, the specific fuel masses, the mean temperatures, and the mean residual mass fractions of the zones in the physical domain are used to define a corresponding set of zones in the multi-zone model. This set of zones is shown in the right-hand side of Fig. 1. The zones are coloured according to their initial temperature.

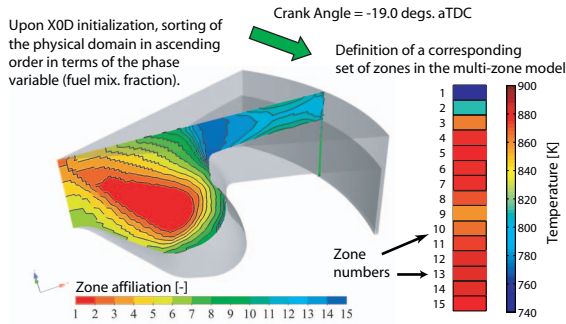


Figure 1: Schematic illustration of the zone initialization in the multi-zone model. Adapted from [10]

Mixing Model In the engine, the mixing is controlled by the turbulence. Obviously, it is desirable to introduce turbulent mixing effects into the multi-zone model solving for the chemistry. This is done as follows: Assuming that, firstly, the combustion chamber is a closed system, meaning that the valves are closed; and secondly, the total mass is constant, then the distribution of the conserved scalars (e.g., the artificial scalar $\tilde{S}$) in the CFD code only changes due to convection and diffusion. The change for the mean artificial scalar $\tilde{S}_i$ from CFD time step $n-1$ to CFD time step n in the individual zones can be described as

$$m_i \cdot \frac{\tilde{S}_i^n - \tilde{S}_i^{n-1}}{\Delta t^n} = \sum_{k=1}^2 \dot{m}_{ik} (\tilde{S}_k^{n-1} - \tilde{S}_i^{n-1}), \quad (9)$$

where Δt^n is the time increment, m_i the mass of zone i , and $\dot{m}_{ik}$ the exchange rate of zone i with neighbouring zone k (see Eqs. (1) and (2)). Since the phase space is one-dimensional, each zone can have up to two neighbours to exchange their scalar quantities with.

Allowing mixing only between neighbouring zones is a logical choice, because transitions in phase space have to be continuous. If a state B is intermediate between two states A and C, then a zone of state A cannot transit to state C without passing through state B during a diffusive process. The zones in phase space are therefore arranged in ascending (or descending) order, as illustrated in Fig. 1. Consequently, neighbouring zone mixing is used in the remainder of the paper. This is analogous to a Representative Interactive Flamelet. In the flamelet equations, the scalar dissipation rate χ is an external parameter that is imposed on the flamelet structure. It can be thought of as a diffusivity in mixture fraction space that accounts for an exchange between adjacent reactive scalars (temperature and species mass fractions) in mixture fraction space. The laminar flamelet equations were derived by Peters [22–24] and integrated into the

concept of Representative Interactive Flamelets by his co-workers [6, 9, 16, 26].

The exchange rate $\dot{m}_{ik}$ is expressed by the average of the neighbouring zones i and k ,

$$\dot{m}_{ik} = 0.5(\dot{m}_i + \dot{m}_k), \quad (10)$$

where $\dot{m}_i$ and $\dot{m}_k$ denote individual exchange rates of zones i and k , respectively. Inserting Eq. (10) into Eq. (9) yields a system of nz unknowns and $nz+1$ equations. The system is overdetermined, because there is no exchange over the boundaries of the phase space and, therefore, the summation of the exchange (see Eq. (9)) over all zones is zero. This constitutes an additional equation. The remedy is to simply fix the value for one of the individual exchange rates $\dot{m}_i$ (e.g., $\dot{m}_1 = 1$). The values for the exchange rates $\dot{m}_{i,k}$ are defined by the two solutions for the mean artificial scalars $\tilde{S}_i$ at CFD time steps n and $n-1$. No matter which value is assigned to one of the individual exchange rates $\dot{m}_i$, it does not change the resulting values for the exchange rates $\dot{m}_{ik}$.

Consistency of Heat Release The chemical source terms $\dot{\omega}_j$ (see Eq. (5)) couple the CFD code AC-FluX to the multi-zone model X0D and keep the heat release consistent between both codes. The fuel mass fraction $\tilde{Y}_{\text{fuel}}$ acts as a progress variable for the heat release. In the CFD code, the average rate of change for the fuel mass $\dot{m}_{\text{fuel},i}$ in zone i is coupled to the gross heat release in the multi-zone model through

$$\dot{m}_{\text{fuel},i} = \frac{\dot{Q}_{\text{ch,X0D},i}}{Q_{\text{LHV}_p}}. \quad (11)$$

In Eq. (11), $\dot{Q}_{\text{ch,X0D},i}$ denotes the gross heat-release rate of zone i that is taken from the multi-zone model. Q_{LHV_p} is the lower heating value of the fuel.

The actual value of the mean fuel mixture fraction in each CFD cell varies from the average value of the zone it belongs to. For this reason, in order to properly distribute the conversion of fuel over the CFD cells, the average rate of change for the fuel mass $\dot{m}_{\text{fuel},i}$ in zone i is weighted with the ratio of the actual mean fuel mixture fraction in CFD cell ijk and the average mean fuel mixture fraction of the corresponding zone i . This yields

$$\dot{m}_{\text{fuel},ijk}^{\text{CFD}} = \frac{\tilde{Z}_{\text{fuel},ijk}^{\text{CFD}}}{\tilde{Z}_{\text{fuel},i}} \cdot \dot{m}_{\text{fuel},i}, \quad (12)$$

where $\dot{m}_{\text{fuel},ijk}^{\text{CFD}}$ denotes the rate of change for the fuel mass in CFD cell ijk and $\tilde{Z}_{\text{fuel},ijk}^{\text{CFD}}$ the actual mean fuel mixture fraction in CFD cell ijk .

The other species (air and products of combustion) which are accounted for in AC-FluX are computed via a one-step global reaction corresponding to the stoichiometry.

Treatment of Source Terms The conservation equation for the mean total enthalpy $\bar{h}$, reading

$$\frac{\partial \bar{\rho} \bar{h}}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_i \bar{h}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho} D_h \frac{\partial \bar{h}}{\partial x_i} \right) + \frac{D \bar{p}}{Dt} + \dot{q}^s - \dot{q}_{\text{wall}}, \quad (13)$$

has two source terms ($\dot{q}^s$ and $\dot{q}_{\text{wall}}$) that need to be accounted for in the multi-zone model X0D.

Vaporization of fuel in the multi-zone model is accounted for by averaging the source term $\dot{\rho}_{\text{fuel}}^s$ in Eq. (7) for each zone in the CFD code. This averaging procedure yields the source term $\dot{\rho}_{ij,j=\text{fuel}}^s$ in Eqs. (1) and (2) and is linked to the source term for the spray in Eq. (13) according to

$$\dot{q}_i^s = \sum_{j=1}^{nsp} \dot{\rho}_{ij}^s \cdot \Delta h_{vj} \quad \text{with} \quad \dot{\rho}_{ij}^s = 0, j \neq \text{fuel}. \quad (14)$$

In X0D, wall heat transfer (see Eqs. (2) and (4)) is described as

$$\dot{q}_{\text{wall},i} \cdot V_i = \dot{Q}_{\text{wall},i} = \sum_{l=1}^{n_{\text{wall}}} A_{\text{wall},l,i} \cdot h_{\text{wall},l,i} (T_i - T_{\text{wall},l}). \quad (15)$$

The area $A_{\text{wall},l,i}$ of wall l belonging to zone i is taken from the CFD solution and updated in the multi-zone model at every CFD time step. The heat transfer coefficient $h_{\text{wall},l,i}$ of zone i to wall l is continuously recalculated based on the CFD solution and updated in the multi-zone model at every CFD time step such that the wall heat transfer in the multi-zone model exactly matches the one in the CFD code. The recalculation of $h_{\text{wall},l,i}$ uses the source term $\dot{q}_{\text{wall}}$ in Eq. (13), also averaged for each zone in the CFD code.

The pressure change in X0D is described by Eq. (3), where the spatial pressure fluctuations are neglected and only the average cylinder-pressure change which is due to the volume change and heat release, is taken into account. The volume change in both codes is computed by using the same slider-crank equation [19].

Thereby, the full interactive coupling of AC-FluX and X0D is accomplished.

COMPUTATIONAL ACCURACY AND EFFICIENCY

The interactively coupled CFD-multi-zone approach efficiently separates the solution of the flow field from the

solution of the chemistry. During one time step of the CFD code, the multi-zone code solves Eqs. (1), (2), and (3) with time steps that can be much smaller, depending on the chemistry. In this way, the time scales of the chemistry and the fluid dynamics are decoupled. Thus, the approach does not need to simplify the highly nonlinear chemistry, allowing for any detailed reaction mechanisms to be used. These mechanisms may also include pollutant formation and destruction. This procedure yields an approach that includes an accurate description of PCCI chemistry with only a small penalty in computational cost, since even during auto-ignition the CFD time step has hardly to be reduced compared to an inert computation of the chemistry.

Decoupling the time scales of the chemistry and the fluid dynamics proved successful in predicting conventional Diesel engine combustion in the framework of Representative Interactive Flamelets (RIF).

In the multi-zone model, 40 differential equations (species mass fractions, temperature, and pressure change; see Secs. "Multi Zone Model" and "Chemistry Model") are solved per zone. Thirteen differential equations are solved in the CFD code (mass, momentum, total enthalpy, active species stream, mean mixture fraction, and artificial scalar conservation, k-epsilon-equations; see Sec. "CFD Code"). The equations in the CFD code are evaluated on each cell. The computations were carried out on a Dell PowerEdge 1950 with two Intel Xeon Dual-Core CPUs with 3.0 GHz (Woodcrest 5160). For this, the approach written in FORTRAN 77 was compiled with the Intel Fortran Compiler 9.1.043. For the interactively coupled CFD-multi-zone approach, the CPU time costs are approximately 24 hours for the thirteen differential equations solved in the CFD code. The CPU time for the multi-zone model depends on the underlying chemical mechanism and on the total number of zones. For $n_z = 15$ zones and the mechanism described in Sec. "Chemistry Model", as is applied here, the computational time for the multi-zone model is about one and a half hours.

EXPERIMENTAL AND NUMERICAL SETUP

EXPERIMENTAL SETUP

Engine At the Institut für Technische Verbrennung at RWTH Aachen University, Germany, experiments were carried out with a 1.9l GM Fiat Diesel engine. This engine is equipped with a second-generation Bosch Common-Rail injection system that was used for all the experiments reported in this study. All relevant engine data are provided in Table 1.

The mounting of the engine on the test bench is shown in Fig. 2.