

A Cycle-Based Multi-Zone Simulation Approach Including Cycle-to-Cycle Dynamics for the Development of a Controller for PCCI Combustion

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ABSTRACT

Subject of this work is a simulation model for PCCI combustion that can be used in closed-loop control development. A detailed multi-zone chemistry model for the high-pressure part of the engine cycle is extended by a mean value model accounting for the gas exchange losses. The resulting model is capable of describing PCCI combustion with stationary exactness. It is at the same time very economic with respect to computational costs. The model is further extended by identified system dynamics influencing the stationary inputs. For this, a Wiener model is set up that uses the stationary model as a nonlinear system representation. In this way, a dynamic nonlinear model for the representation of the controlled plant Diesel engine is created.

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, 19, 30]. 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 [8]. 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. Sophisticated closed-loop control of the combustion process is one means to overcome this difficulty. Against this background, this paper deals with a first step towards the development of a controller for the PCCI combustion process.

The most important characteristics for the operation of an internal combustion engine are the engine's load and its combustion efficiency. The former is directly dependent on the indicated mean effective pressure (IMEP), the latter can be characterized by the centre of combustion, where 50 % of the total injected fuel mass is burned (CA50). The engine's load is set by the driver in an automobile application. For CA50, a set point can be determined which is dependent on the operating point and gives the best combustion efficiency. These two variables are the main focus of the controller to be developed. For influencing the process, the start of injection (SOI), the external EGR rate, and the total fuel mass injected are suitable actors.

In the recent past, several efforts have been reported in the literature that aim at controlling engine combustion. Among them, one can mention [5, 18, 20, 29, 31]. The standard procedure for creating a controller includes the modeling part as the first step [1, 6, 28]. Often this model differs in several aspects from models widely used for gathering a deeper understanding of combustion details, like three-dimensional computational fluid dynamics (CFD) models [4, 7, 24, 25]. From the viewpoint of automatic control, the dynamics describing the dependency of the system's outputs (IMEP, CA50) on the actors (SOI, external EGR rate, and total fuel mass injected) is of highest priority. Nevertheless, stationary exactness is important, too. Another requirement is an acceptable calculation speed, as it often is necessary to test the controller in dynamic closed-loop simulations.

This paper presents a new approach to the development of a simulation model for the use in closed-loop control development. The model is based on a recently introduced multi-zone model for PCCI combustion that was derived from a detailed CFD model. It covers the nonlinear dependencies within the high-pressure part of the engine cycle with stationary exactness. This model is extended by a physically inspired description of the gas exchange part of the engine cycle. For the use in closed-loop simulations the system's dynamics have to be covered. For this reason, the stationary model is further extended by identified system dynamics influencing the stationary inputs. In this manner, a stationary exact model is extended to a Wiener-type model with a static part describing the nonlinearities and an upstream part describing the system's dynamics. This novel proceeding brings the detailed knowledge from combustion simulation tools into closed-loop control and establishes a broad field of possibilities for testing completely new controlled process variables.

The paper is arranged as follows: The first section discusses the combustion modeling approach employed in the current investigation. The fundamental theory and assumptions underlying the multi-zone chemistry model are reviewed. Further on, its stationary validation is presented. In the next section, the physically inspired description of the gas exchange part of the engine cycle is put forward. Following this, the system's dynamics are identified. Finally, the conclusions and major findings from the study are summarized and an outlook to future work is given. Frequently used definitions, acronyms, and abbreviations are included at the end of the paper, following the references.

COMBUSTION MODEL FORMULATION

Crucial for reacting turbulent flows is the modeling of the chemistry. Here, a multi-zone chemistry model is employed. This multi-zone chemistry model covers the nonlinear dependencies within the high-pressure part of the engine cycle with stationary exactness. The methodology and its validation are outlined in this section.

MULTI-ZONE MODELING FRAMEWORK Recently, Barths et al. [3] developed a consistent mixing model for the two-way-coupling of CFD codes and zero-dimensional multi-zone codes, yielding a hybrid CFD/zonal modeling approach for HCCI chemistry that aims at reducing the computational overhead for large chemical mechanisms. There, all aspects except chemical kinetics were computed using three-dimensional CFD, and CFD cells were binned into a relatively small number of zones for the chemistry calculations. In [3], each CFD cell was binned into one of 27 zones based on its fuel mixture fraction, dilution, and total enthalpy. Issues within the two-way-coupling included maintaining thermodynamic consistency between the two representations and interactions among zones. Following from there, an interactively coupled CFD-multi-zone approach was presented that can be used to simulate HCCI combustion [11]. Felsch et al. [13] applied this interactively coupled CFD-multi-zone approach for various PCCI operating conditions in a 1.9l FIAT GM Diesel engine. In the same work, the interactively coupled CFD-multi-zone approach was systematically reduced towards a computationally efficient stand-alone multi-zone model. For this, the multi-zone model was decoupled from the CFD code. In the framework of the interactively coupled CFD-multi-zone approach, all relevant information fed from the CFD code to the multi-zone model was identified. This information was then modeled within the decoupled stand-alone multi-zone model. The validity of the reduction was limited to the investigated 1.9l FIAT GM Diesel engine that is also subject of the present work. The stand-alone multi-zone model showed a significant advantage with respect to computational costs. Due to its strict derivation, it was at the same time nearly as predictive as the interactively coupled CFD-multi-zone approach.

The theoretical background of the stand-alone multi-zone model is briefly summarized in the following. Thereby, it is assumed that essential information obtained from preceding simulations with the interactively coupled CFD-multi-zone approach or throughout the reduction process, respectively, is available. For detailed information, the reader is referred to [13].

MULTI-ZONE CHEMISTRY 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. [16] and Felsch et al. [12].

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

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

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

and

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

In Eq. (1), Y_{ij} denotes the mass fraction of species j in zone i , and $\dot{\omega}_{ij}$ is the corresponding chemical source term. $\dot{\rho}_{ij}^s$ 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 mass exchange between the zones, where $\dot{m}_{ik}$ is the rate at which mass is transported between zones i and 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. 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.

The mixing in the multi-zone model is accounted for by allowing the different zones to exchange mass and energy with each other, in addition to the interaction through the pressure. They exchange their scalar quantities (species composition and enthalpy) based on the rate at which they exchange their mass. The mass of each zone is kept constant and the model can accommodate any number of zones.

Heat Transfer to the Walls 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. $A_{wall,l,i}$ is 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 heat transfer coefficient $h_{wall,l,i}$ is modeled with the Woschni correlation [34],

$$h_{wall,l,i} = h_{wall} = 3.26 \cdot b^{-0.2} \cdot p^{0.8} \cdot T_{av.}^{-0.53} (C_1 \cdot v_{piston})^{0.8}, \quad (5)$$

where b is the bore of the engine, p the mean cylinder pressure, $T_{av.}$ the average in-cylinder temperature, and v_{piston} the mean piston speed. The constant C_1 is adjustable and is set to 0.5. Since the average in-cylinder temperature $T_{av.}$ is used within the Woschni correlation and $h_{wall,l,i}$ does not depend on any specific wall, the heat transfer coefficient is equal for all zones, leading to $h_{wall,l,i} = h_{wall}$.

For the specific engine investigated, the area $A_{wall,l,i}$ of wall l belonging to zone i has to be taken from a preceding simulation with the interactively coupled CFD-multi-zone approach mentioned above. Then, this information can be incorporated into a successive simulation with the stand-alone multi-zone model.

Fuel Injection and Vaporization A preceding simulation with the interactively coupled CFD-multi-zone approach also allows for determining the amount of fuel that is injected and vaporizes in each CFD zone. This information can then be incorporated into a successive simulation with the stand-alone multi-zone model (see source term $\dot{\rho}_{ij}^s$ in Eqs. (1) and (2)).

Mixing Model The mixing model within the stand-alone multi-zone model assumes that the mass exchange rate $\dot{m}_{ik}$ of zone i with neighbouring zone k (see Eqs. (1) and (2)) is proportional to the wall heat transfer coefficient h_{wall} and the area A both zones share [16]. This is an analogy to the well known empirical Lewis law, which assumes a similarity between heat and mass transfer [2]. The corresponding equation reads

$$\dot{m}_{ik} = r_{MB} \cdot A \cdot \frac{m_i + m_k}{(m_i \bar{c}_{pi} + m_k \bar{c}_{pk})} \cdot h_{\text{wall}} \cdot \quad (6)$$

In Eq. (6), $\bar{c}_{pi}$ is the average heat capacity at constant pressure of zone i . r_{MB} is a parameter that is adjusted to yield the desired level of mixing. In this study, r_{MB} is set to 75.0 during compression and expansion. During injection r_{MB} linearly increases until 500.0. After end of injection r_{MB} linearly decreases again back to 75.0. The area A is computed from the volumes V_i and V_k of the two zones i and k according to

$$A = 4\pi \left[\frac{3}{4\pi} (V_i + V_k) \right]^{\frac{2}{3}}. \quad (7)$$

Chemistry Model A major aspect in modeling 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. [23]. The NO-submechanism, which is part of the full mechanism, is the extended Zeldovich mechanism [17].

COMPUTATIONAL ACCURACY AND EFFICIENCY The stand-alone multi-zone model does not solve for the solution of the flow field. This yields a significant advantage in computational costs in comparison to three-dimensional CFD modeling approaches. The run time for the stand-alone multi-zone model is approximately 3.3 minutes per high-pressure engine cycle for a simulation with 15 zones on a Dell PowerEdge 1950 with two Intel Xeon Dual-Core CPUs with 3.0 GHz (Woodcrest 5160). For such a simulation, the stand-alone multi-zone model written in FORTRAN 77 was compiled with the Intel Fortran Compiler 9.1.043. However, modeling the CFD information according to the procedure outlined above may reduce the accuracy of the simulation outcome. A detailed discussion of the computational accuracy and efficiency of the stand-alone multi-zone model can be found in [13].

STATIONARY VALIDATION

Experimental Setup 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. All relevant engine data are provided in Table 1.

Engine type:	Four-cylinder research engine
Displacement volume:	1910 cm ³
Bore:	82.0 mm
Stroke:	90.4 mm
Bore distance:	90.0 mm
Cylinder block height:	236.5 mm
Connecting rod length:	145.0 mm
Compression height:	46.5 mm
Valve diameter I/E:	28.5/25.5 mm
Compression ratio:	17.5:1
Output @ engine speed:	110 kW/4000 rpm
Torque @ engine speed:	315 kW/2000 rpm
Idle speed:	850 rpm
Maximum speed:	5100 rpm
Injection System:	7-hole injector
Included spray angle:	100.0 degrees
Hole diameter:	0.141 mm
Flow number:	440 cm ³ /30s @ 100 bar
Swirl number:	2.5
Fuel:	Diesel

Table 1: GM Fiat engine specifications

The mounting of the engine on the test bench is shown in Fig. 1. A more detailed description regarding the engine, the test cell equipment, and injection rate measurements can be found in Vanegas et al. [33].

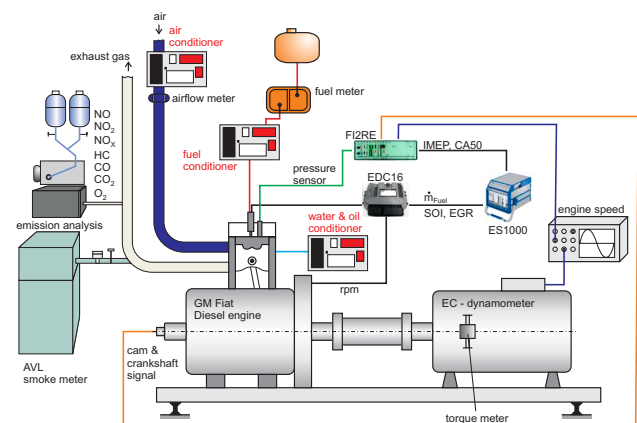


Figure 1: Engine test bench

The engine operating conditions are summarized in Table 2. The engine was operated at part-load conditions with a speed of 2000 rpm and an external EGR rate of

15, 30, or 45 %, respectively. Ten variations of start of injection (SOI) were investigated for each external EGR rate, leading to 30 different experiments. The SOI variation started at -45.7 degs. CA aTDC and lasted until -0.7 degs. CA aTDC with a time shift of 5.0 degs. CA between two consecutive SOIs. For all cases, the total fuel mass injected was 10.2 mg/cycle, with an injection duration of 8.8 degs. CA. Two additional SOI variations were carried out with an external EGR rate of 30 % and a reduced total fuel mass injected of 6.8 mg/cycle, or an increased total fuel mass injected of 13.6 mg/cycle, respectively, leading to another 20 different experiments. In these cases, the injection duration was 5.9 or 11.7 degs. CA, depending on the total fuel mass injected. The rail pressure was 700 bar for all 50 cases.

Engine speed:	2000 rpm
Rail pressure:	700 bar
Fuel mass injected:	6.8, 10.2, or 13.6 mg/cycle
Relative air/fuel ratio:	between 5.3 and 1.6
External EGR rate:	15, 30, or 45 %
Start of Injection (SOI):	-45.7 degs. CA aTDC -40.7 degs. CA aTDC -35.7 degs. CA aTDC -30.7 degs. CA aTDC -25.7 degs. CA aTDC -20.7 degs. CA aTDC -15.7 degs. CA aTDC -10.7 degs. CA aTDC -5.7 degs. CA aTDC -0.7 degs. CA aTDC

Table 2: Engine operating conditions

Numerical Setup Computations with the stand-alone multi-zone model were performed for all 50 cases presented above. All computations started from intake valve closure (IVC) at -165.6 degs. CA aTDC and ended at exhaust valve opening (EVO) at 149.1 degs. CA aTDC. The starting solution at IVC was initialized with pressure and temperature taken from the experiments. The internal EGR rate was assumed to be 5 %. The wall temperatures were set based on experimental experience and held constant during the simulations. A sensitivity study revealed that beyond $nz = 15$, the change of the ignition timing and the overall heat-release rate was insignificant. Thus, a number of zones of $nz = 15$ zones was chosen for all subsequent simulations.

In the next subsection, the stand-alone multi-zone model is exemplarily validated against five selected operating conditions. This includes five variations of SOI (-35.7, -30.7, -25.7, -20.7, and -15.7 degs. CA aTDC) at an external EGR rate of 30 %, which will be referred to as timings 1, 2, 3, 4, and 5 (TS-1, TS-2, TS-3, TS-4, and TS-5) in the remainder of the paper.

TS-3 was used as a calibration case for incorporating information from the interactively coupled CFD-multi-zone approach into the stand-alone multi-zone model ($\dot{\rho}_{ij}^s$ and $A_{wall,l,i}$, see Eqs. (1), (2), and (4)). The information obtained for TS-3 from the simulation with the interactively coupled CFD-multi-zone approach was used for all cases investigated with the stand-alone multi-zone model. This introduces a small error into the stand-alone multi-zone model simulations for TS-1, TS-2, TS-4, and TS-5. However, this error is small, since the calibration conditions of TS-3 do not deviate significantly from the conditions of the other timings.

Modeling Results Figure 2 compares the pressure curves and the corresponding indicated mean effective pressures for the high-pressure part of the engine cycle ($IMEP_{HP}$) obtained from the simulations with the stand-alone multi-zone model with the results from the experiments for the complete SOI variation. It becomes evident that with retarded SOI timings the maximum pressure peak decreases, while the $IMEP_{HP}$ increases. For all five cases, the simulations are in good agreement with the experiments. There is only a slight overestimation of the maximum peak pressure and a slight underestimation of the $IMEP_{HP}$ in all simulations. The qualitative trends are reproduced well by the simulations.

Figure 3 shows the crank angles at which 10 % (CA10) and 50 % (CA50) of the injected fuel mass is burned for all simulations and experiments. While CA50 is predicted almost perfectly, the simulated CA10 has a slight but acceptable deviation from some of the experimental results.

Figure 4 summarizes the CO emissions in g/kg fuel in the exhaust gas and the combustion efficiency in percent for the complete SOI variation. The CO emissions, which are rather challenging to predict, are slightly overestimated in the simulations. This leads to an underestimation of the combustion efficiency, since the simulated HC emissions (not shown here) are roughly of the same order of magnitude as the experimentally obtained ones for all cases. Overall, the qualitative and quantitative agreement over the whole SOI variation is reasonable for both CO emissions and combustion efficiency.