Predicting auto-ignition characteristics of RCCI combustion using a multi-zone model

PCCI combustion modeling with a multi-zone approach including inter-zonal mixing

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Abstract Premixed charge compression ignition (PCCI) is a clean and efficient alternative for classical diesel combustion. The concept of PCCI combustion is associated with early injection of the fuel whilst applying high exhaust gas recirculation (EGR) levels and operation with a highly lean mixture such that ignition takes place (well) after the injection event. Thus, it is possible to reduce soot and oxides of nitrogen (NO_x) emissions simultaneously. PCCI combustion is analyzed using a multi-zone model. In the multi-zone model, chemical mechanisms which are much more detailed compared to those used in computational fluid dynamics (CFD) approaches can be introduced directly. The CFD model is still used to predict the initial fuel stratification in the cylinder which is important to improve the quality of the model. For the analysis, dedicated experiments with n-heptane are used to evaluate the results of the model. In such a multi-zone model, 10 zones prove to be sufficient to describe the stratification with adequate resolution. It is observed that different fuel distributions have a large influence on the emissions when there is no mixing between the zones. To overcome this dependence, a basic inter-zonal diffusive

mixing is applied. The level of mixing is estimated with a sensitivity study. When the inter-zonal mixing is included, emission results become much less sensitive to the crank angle (CA) at which the charge stratification is sampled and the simulation is initialized.

Keywords Premixed charge compression ignition; multi-zone modeling; stratification; detailed chemistry.

1 Introduction

Since emission regulations become more stringent, new combustion concepts should be developed to meet these emission standards. Although compression ignition (CI) engines lead to lower carbon dioxide (CO_2) emissions due to their higher efficiency compared to spark ignition (SI) engines, they suffer from high oxides of nitrogen (NO_x) and soot emissions [1]. Premixed charge compression ignition (PCCI) is a promising alternative for diesel combustion which has the potential of combining the superior emission levels of SI and high efficiency of conventional CI engines.

PCCI combustion avoids circumstances which result in high NO_x and soot emission [1-3]. Very low NO_x emissions are achieved in this concept by operating with a highly diluted mixture which lowers the in-cylinder temperature, resulting in low-temperature combustion (LTC). On the other hand, fuel-air mixing is improved by applying much earlier injection timings in combination with high exhaust gas recirculation (EGR) levels. This lowers local equivalence ratios and thus results in very low soot emissions.

As the fuel is injected early in the compression stroke, the fuel injection and heat release events have no overlap which makes the combustion process primarily controlled by chemical kinetics. However, when the heat release event is uncoupled from fuel injection, combustion timing control in case of auto-ignition becomes a difficult issue in engine development and calibration. To decrease development and calibration time and costs, the significance of numerical modeling increases even more.

As PCCI-like combustion is mainly governed by auto-ignition and not by flame propagation [4-7] multi-zone approaches are believed to be a feasible approximation for this combustion regime. The main advantage of multi-zone models over computational fluid dynamics (CFD) tools is that more detailed chemical mechanisms can be applied directly. Therefore multi-zone modeling has been applied extensively in engine community [8-16]. In those studies, the complex flow phenomena are ignored. This is a major drawback since emissions are severely affected by the level of stratification and flow induced mixing processes. This deficiency is overcome by fully coupling of the multi-zone model with a CFD model [17-24]. In such a two-way coupled model, a zone in the CFD model corresponds to a zone in the multi-zone model. The chemistry is solved in the multi-zone model, the heat release is transferred to the CFD model, the transport equations are solved by the CFD model, and mixture compositions are fed back to the multi-zone model. As both models interact at each time step, the computational effort is increased remarkably.

In this study, a more pragmatic approach is pursued. The purpose is to estimate the stratification level with the utilization of a CFD model while keeping the computational effort at reasonable levels. Besides, a basic mixing model is applied in the multi-zone model (XCCI code, [25]). The diffusion term consists of the gradient of the species or temperature over the zonal boundaries, a laminar diffusion coefficient and a turbulent diffusivity factor as explained further on. A sensitivity study is performed to determine this turbulent diffusivity factor. The XCCI-CFD interaction is not taken into account in a two-way coupled manner. Only the zonal fuel distribution (stratification) which is needed as the initial condition for the model is determined by the CFD model.

Dedicated PCCI combustion experiments are conducted on a research heavy duty (HD) diesel engine using n-heptane as a fuel. This fuel has a cetane number that is comparable to that of regular diesel fuel but is much more volatile. The main reason for using this specific fuel, instead of regular diesel, is to minimize the modeling uncertainty with respect to the fuel chemistry which is known for n-heptane but not for diesel. The experimental results are compared with the XCCI code.

In the following section, the modeling approach is described including the XCCI-CFD interaction. Then, the experimental setup is presented. In the results part, the effects of different modeling parameters, i.e. the number of zones, chemical mechanisms, inter-zonal mixing and stratification level, are discussed.

2 Modeling Approach

The XCCI code is a multi-zone code developed to perform PCCI/HCCI (homogeneous charge compression ignition) combustion simulations using a wide variety of detailed chemical models. The multi-zone feature is established by dividing the cylinder volume into a number of zones. In this study the zones are arranged as rings around one central cylinder and the zones interact with the neighboring zones. Consequently only the outer zone has contact with the cylinder walls whereas all the zones are in contact with the cylinder head and the piston depending on their volumetric ratios. The geometrical arrangement has most impact on the effect of the cooling model that is applied. In the following sections the mathematical and chemical models as well as the initialization of the model are presented.

2.1 Mathematical Model

Energy conservation in the XCCI code is based on the first law of thermodynamics for open systems and the equation yields,

$$m_z c_v \frac{dT_z}{dt} = -\sum_{i=1}^{N_s} e_i \frac{dm_{z,i}}{dt} + \dot{Q}_z + \dot{Q}_{z,T} - p\frac{dV_z}{dt} + \sum_{i=1}^{N_s} \dot{m}_{z,i}^{in} h_i(T_{in}) + \sum_{i=1}^{N_s} \dot{m}_{z,i}^{out} h_i(T_z) + \sum_{i=1}^{N_s} \dot{m}_{z-1,i}^{D} h_i\left(T_{z'}\right) + \sum_{i=1}^{N_s} \dot{m}_{z+1,i}^{D} h_i\left(T_{z''}\right) \quad (1)$$

where subscripts z and i are used to denote the zone and species number, respectively. N_s is the number of species, m_z is the total zone mass, T_z is the zone temperature, V_z is

the zone volume and p is the pressure. $m_{z,i}$, e_i and h_i are the mass, internal energy and enthalpy of species i, respectively. Heat capacity is the mass-weighted average, $c_v = \sum Y_i c_{v,i}$. $\dot{Q}_z$ is a lumped quantity describing the heat transfer rate due to heat loss and evaporative cooling during the fuel injection. $\dot{m}_{z,i}^{in/out}$ is the mass flow through the boundaries. T_{in} is the temperature of the intake flow. Similarly the enthalpy flow associated with mass-diffusion is captured in the last two terms on the right hand side. The actual values for $T_{z'}$ and $T_{z''}$ depend on the direction of the fluxes. The term $\dot{Q}_{z,T}^{D}$ on the right hand side represents a basic heat conduction model between the zones,

$$\begin{aligned} \dot{Q}_{z,T}^{D} &= \int_z \vec{q} \cdot \vec{n} dA \\ &= A_{z,z-1} C_t \lambda \left(\frac{\Delta T}{\Delta R} \right)_{z,z-1} + A_{z+1,z} C_t \lambda \left(\frac{\Delta T}{\Delta R} \right)_{z+1,z} \end{aligned} \tag{2}$$

where C_t is a constant which refers to the turbulent diffusivity factor. The same constant is used for all zones and the coefficient is not a function of time. $A_{z,z'}$ is the zone boundary area between zones z and z', λ is the laminar conduction coefficient.

The vaporizing fuel is also treated according to the 1st law of thermodynamics for open systems. The heat loss due to evaporation is taken into account by the enthalpy differences between liquid and vapor phases of the fuel at a certain temperature.

The change of mass of the species in the system is introduced by the chemical reactions (M1), by the intake and exhaust mass flow of each zone (M2) and by the mass exchange through the boundaries due to the zonal mixing (M3),

$$\frac{dm_{z,i}}{dt} = \underbrace{V_z\left(M_i\sum_{j=1}^{N_r}\nu_{ij}\omega_j\right)}_{M1} + \underbrace{\dot{m}_{z,i}^{in/out}}_{M2} + \underbrace{\Delta\dot{m}_{z,i}^{D}}_{M3} \tag{3}$$

Subscript j is used to denote the reaction number, N_r is the number of reactions, M_i is the molar mass of species i, ω_j is the reaction rate of reaction j. Furthermore, ν_{ij} is the stoichiometric coefficient of species i in reaction j. M3 equals

$$\begin{aligned}\Delta\dot{m}_{z,i}^{D} &= \int_z \rho\vec{V}_i\cdot\vec{n}dA \\ &= \dot{m}_{z-1,i}^{D} + \dot{m}_{z+1,i}^{D} \\ &= A_{z,z-1}C_t\frac{\lambda}{c_p Le_i}\left(\frac{\Delta Y_i}{\Delta R}\right)_{z,z-1} + A_{z+1,z}C_t\frac{\lambda}{c_p Le_i}\left(\frac{\Delta Y_i}{\Delta R}\right)_{z+1,z}\end{aligned} \tag{4}$$

Each zone has its own temperature (T_z), volume (V_z) and mass of species ($m_{z,i}$) while the pressure (p) is the same for all zones. The zones are coupled to each other by the equation of state,

$$pV_z = m_z\frac{R_u}{M_z}T_z \tag{5}$$

where R_u is the universal gas constant and M_z is the zone average molar mass. The set of equations is closed by the constraint that the summation of zone volumes is equal to the total volume at time t. Initially, the zones have equal volumes, while during the simulations, the zones expand or shrink (i.e. the volume of each zone changes) depending on the local conditions.

$$\sum_{z=1}^{N_z}V_z = V_{(t)} \tag{6}$$

In the model, the heat transfer to the cylinder walls, cylinder head and piston can be taken into account by different heat loss mechanisms. In this study, the modified Woschni correlation by Assanis [26] is applied during the simulations. The heat loss mechanism affects the evolution of a simulation. Since the outer zone has contact with the cylinder walls, the heat loss from the outer zone is larger than the other zones and this makes the temperature of the outer zone lower than the rest especially prior to ignition.

In short, the unknowns that need to be solved in the model are pressure, p, and for each zone the temperature, the volume and the mass of each species, viz. V_z, T_z, $m_{z,i}$. Since detailed chemical mechanisms are used, the set of coupled non-linear equations is large and typically stiff. Consequently, an efficient and reliable solver is applied (i.e. DASSL [27]).

2.2 Chemical Model

Since the chemistry of the commercially available fuels is not yet comprehended, surrogate fuels receive a lot of attention lately. Surrogate fuels are based on primary reference fuels (PRF's), e.g. n-heptane and iso-octane (others also exist, see [28]) augmented with additional sub mechanisms (e.g. toluene) to model the fuel chemistry over a wider range of conditions.

In this paper three chemical mechanisms are included. The first one is a well-known semi-detailed gasoline surrogate mechanism (Andrae [29]) based on a skeletal n-heptane/iso-octane PRF model to which toluene, diisobutylene and ethanol mechanisms are added. The mechanism consists of 137 species and 633 reactions. The second mechanism is a more detailed n-heptane mechanism of Seiser et al. [30]. It is based on the detailed n-heptane mechanism of Curran et al. [31] (556 species and 2540 reactions) reduced systematically to 159 species and 770 reactions. The last mechanism (48 species, 248 reactions) is derived from the mechanism of Peters et al. [32] by replacing C1-C3 sub-mechanism with that of GRI3.0 [33].

2.3 Initial Conditions

The simulations are initialized at the moment of Intake Valve Closing (IVC) by setting inlet temperature, inlet pressure, total cylinder mass and mixture composition (calculated from EGR level) from the experimental data. Initial conditions are the same for all zones. All zones have the same temperature, volume as well as mixture composition during the start of the simulation. Mixture composition differs between the zones due to fuel injection. Different amounts of fuel are injected in each zone defined by a set stratification level. In this study, stratification is accounted for with respect to the fuel/air ratio. It can obviously not be measured in the full metal engine. Thus, the stratification level is obtained from CFD model results of the research engine,

developed in StarCD. The CFD model of the engine has been validated in another study [34]. Here, it is used to simulate the evolution of the fuel distribution as a function of the injection timing. For illustration, the computed fuel contours for a SOI (start of injection) of 50°CA (degrees crank angle) bTDC (before top dead center) case are presented in Figure 1.

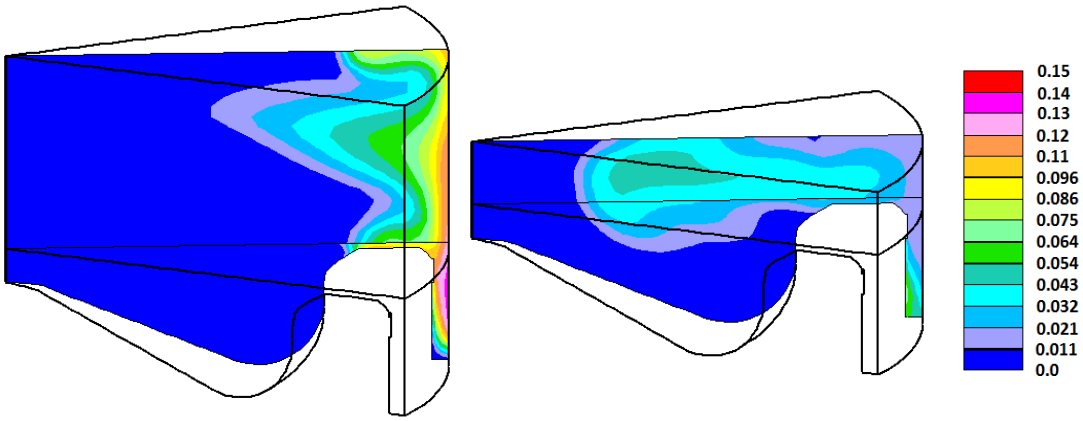

Fig. 1 Sample fuel mass fraction levels at different crank angles (40° and 15°CA bTDC, respectively) for an early injection case (SOI=50°CA bTDC, EOI=43°CA bTDC).

To determine different levels of stratification in the multi-zone simulations the actual fuel distribution per simulated case is sampled at various crank angles (Figure 2(a)). In this approach a direct mapping is applied at a sampling moment from 3D to 1D by sorting all the cells with respect to their fuel mass fractions. In other words, the topology of the distribution is disregarded. From that a monotonic distribution is

constructed, where the richest zone corresponds to the outer zone. To test the approximation a simulation is performed where the radial (i.e. spatial) locations are taken into account by summing the amount of fuel in each cell belonging to each zone. Consequently, the distribution is not monotonic anymore. The results were quite similar. The reason for this is that the richest cells always exist near the cylinder wall as it is illustrated in Figure 1. No matter which method is applied, the richest zone corresponds to the outer zone. The outer zone is the main contact with the cylinder wall and it suffers from the largest heat loss. As a result the outer zone is the main source of CO emissions and the details of the distribution does not play a major role.

The normalized fuel fraction for injection is defined based on this distribution. Since the total amount of injected fuel is already known, the injected fuel mass per zone is obtained by simply multiplying this fraction with the total fuel mass which is 50 mg/cycle. The corresponding amount of fuel is then injected in each zone to obtain an equivalent stratification (Figure 2(b)). Obviously, the stratification is an important parameter on which results are expected to depend. Thus, different sampling moments are chosen to perform a sensitivity study.

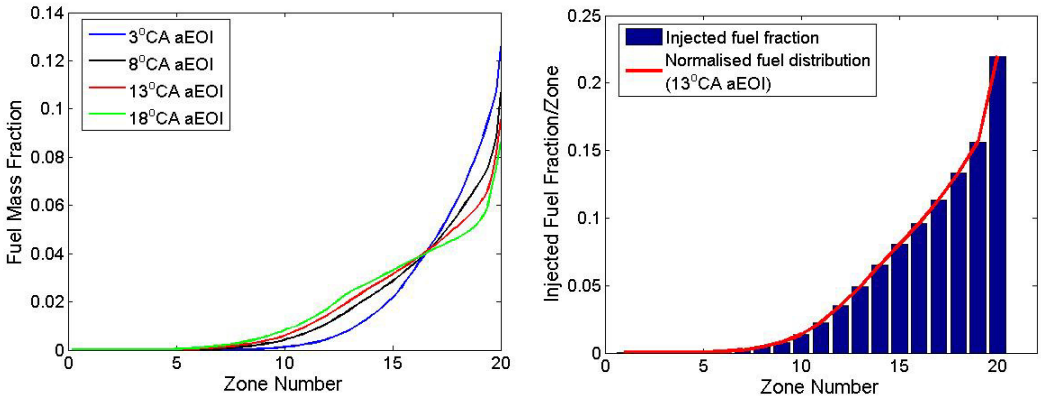

Fig. 2 (a) Typical fuel distributions, derived from CFD, applied in the multi-zone model. (b) Discretised injected fuel fraction for distribution at 13°CA aEOI (SOI=30°CA bTDC).

3. Experimental Setup and Measurement series

3.1 Measurement Program

In a short term scenario, PCCI combustion will in practice only be used in the low load part of the engine operating range, with conventional CI combustion at higher loads. The implication of this scenario is that engine hardware design would be very close to that of current modern diesel engines, with the effective compression ratio possibly made load dependent through implementation of variable valve actuation. Therefore optimizing operating conditions should focus on parameters like EGR level, intake temperature, intake pressure and injection timing.

In the measurements the effects of these operating conditions have been investigated on ignition delay, or available mixing time, combustion phasing and maximum pressure rise rate.

3.2 Experimental Engine Setup

The CYCLOPS is a dedicated engine test rig, see Table 1 and [35], based on a DAF XE 355 C engine. Cylinders 4 through 6 operate under the stock engine control unit and together with a Schenck W450 dynamometer they are merely used to control the crankshaft rotational speed of the test cylinder, i.e. cylinder 1, in which combustion phenomena and emission formation can be studied. Apart from the mutual cam- and crankshaft and the lubrication and coolant circuits, the test cylinder operates autonomously from the propelling cylinders.

Table 1 CYCLOPS specifications

Base engine	6 cylinder HDDI diesel
Cylinders	1 isolated for combustion
Bore [mm]	130
Stroke [mm]	158
Compression ratio [-]	12:1
Bowl shape	M-shaped
Bowl diameter [mm]	100

Fed by an Atlas-Copco air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. Non-firing cylinders 2 and 3 function as EGR pump

cylinders, the purpose of which is to generate adequate EGR flow, which is cooled both up- and downstream of the pump cylinders.

Fuel to cylinder 1 is provided by a double-acting air-driven Resato HPU200-625-2 pump and a accumulator is placed near (~0.2 m) the fuel injector to mimic the volume of a typical common rail. The prototype common rail injector used has a nozzle with 8 holes of 0.151 mm diameter with a cone angle of 153 degrees.

For measuring gaseous exhaust emissions a Horiba Mexa 7100 DEGR emission measurement system is used. All quasi steady-state engine data are recorded by means of an in house data acquisition system (TUeDACS) and a SMETEC Combi crank angle resolved data acquisition system is used to record and process cylinder pressure data. For more information on the experimental setup and procedures, the reader is referred to [35,36].

3.3 Measurement Matrix

For all experiments, a number of parameters is chosen to be kept constant over the whole series. To investigate the effects of several parameters on PCCI combustion, the operating conditions given in Table 2 are tested, using n-heptane as the fuel.

Table 2 Operating conditions

Engine Speed	1200 rpm
Fuel injection pressure	1500 bar
Fuel temperature	307 K
Intake air temperature	300 K

Injection durations	900 – 1200 – 1600 μs
Intake pressure levels	1.25 – 1.5 bar
EGR levels	0 - 15 - 40 - 50 - 60 wt %.

For every combination of operating conditions under investigation, a sweep of start of actuations (SOA) of the injector is performed. Starting from conventional CI timings, SOA is advanced at five degree increments, skipping SOAs at which combustion is not acceptable. Acceptable combustion in this aspect is defined by both engine hardware limitations and combustion quality targets.

4 Results

The main purpose of this study is to analyze the effect of modeling parameters rather than the effect of engine operating conditions. It is aimed to develop and present a predictive model together with its sensitivities to sub-models. Thus, one operating point for each variable operating condition is chosen (Injection duration is 900 μs, intake pressure is 1.25 bar and EGR level is 50%). The only difference between the studied cases is the start of injection. The start of injection is varied from 50^{o}CA bTDC to 25^{o}CA bTDC with five degree intervals. The numerical results will be analyzed with respect to the combustion phasing and carbon monoxide (CO) emissions. CO emissions are utilized especially to judge the significance of inter-zonal mixing. First the sensitivity of the results to the number of zones and the applied chemical mechanism

will be determined. After that with the optimal settings the effect of inter-zonal mixing and, related to that, the degree of stratification are investigated.

4.1 Effect of number of zones

The advantage of the multi-zone model compared to a single-zone model is the ability to introduce stratification, i.e. inhomogeneity in the mixture. Nevertheless, the adequate number of zones should be determined. Here, the results of 1, 5, 10, 20 and 40 zones are compared. The chemical mechanism of Andrae is used for these simulations. Two arbitrarily chosen cases are presented for the sensitivity analysis with respect to the number of zones (Table 3). In order to analyze the pure effect of number of zones, heat loss to cylinder walls and zonal mixing are ignored here.

Table 3 Sampling moments used for the effect of the number of zones analysis.

SOI (^{o}CA bTDC)	Sampling Moment (^{o}CA bTDC)	Nomenclature
30	5	D1
50	30	D2

When total CO emissions (Figure 3(a)) are compared, the effect of number of zones is clear. As expected, the single zone case deviates the most. In a single zone simulation, the cylinder volume is totally homogeneous which is not realistic. It is merely introduced as a reference. As the mixture is lean (excess air ratio (λ) = ~2.4) and totally homogeneous, complete combustion occurs resulting in zero CO emissions.

When more zones are introduced, the results converge to a common value for 10, 20 and 40-zone cases. The difference between the multiple zone cases is due to the fact that for this setting, more fuel is injected in outer zones where there is heat loss to the cylinder walls. Due to the higher amount of incomplete combustion, CO emissions become higher especially for the five zone simulation. Similar conclusions are drawn when NO_x and unburned hydrocarbons (UHC) emissions are studied. From this observation it is concluded that 10 zones are sufficient to describe the effect of stratification for emissions with adequate resolution.

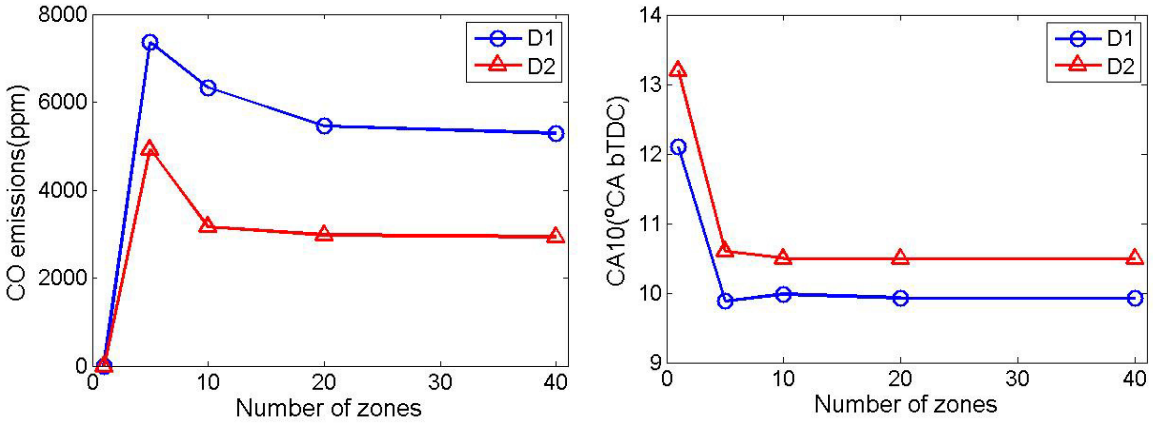

Fig. 3 (a) CO emissions (b) CA10 as a function of number of zones. See Table 3 for injection timings and sampling moments of the cases.

In the next step, the combustion phasing results are compared (Figure 3(b)). CA10, defined as the crank angle where 10% of the total heat is released, is used to quantify

the timing of start of combustion, which in its turn can be utilized to indicate the combustion phasing. Here, the excess amount of O_2 in the homogeneous charge for the single zone case initiates combustion earlier. Still, the effect of the number of zones is limited with the difference between the extreme cases less than 0.5°CA for multiple zone cases. A similar insensitivity is observed for the burn duration. Therefore both from the emission results as well as the results from the combustion phasing it appears that 10 zones are sufficient. These findings hold also for a broader range of operating conditions. Thus 10 zones will be used as default for the rest of the study.

4.2 Effect of chemical mechanisms

The reactions and the species formed during those reactions are represented by chemical mechanisms. The simulations are performed with the stratification CFD data sampled at crank angles of 13°CA aEOI for the three different reaction mechanisms.

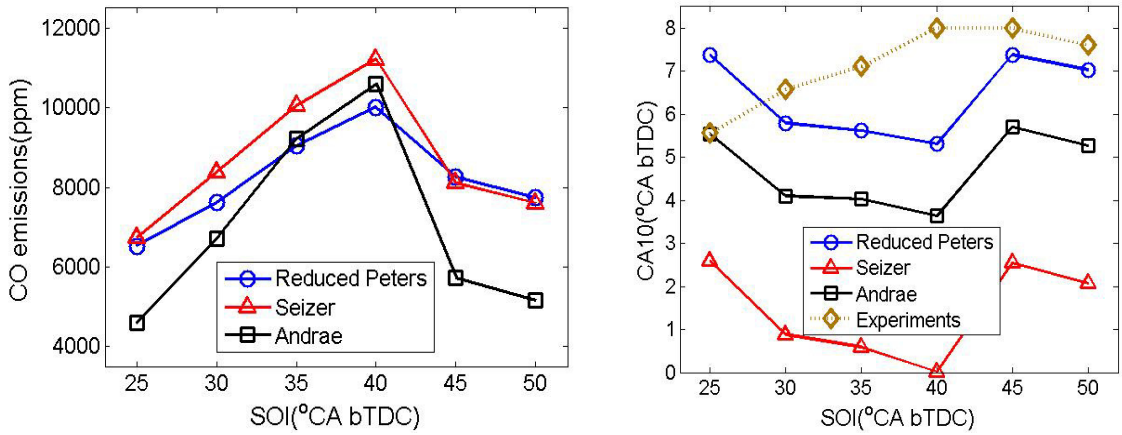

Fig. 4 (a) CO emissions (b) CA10 as a function of SOI for three different reaction mechanisms.

It is concluded from Figure 4(a) that using different mechanisms has a large influence on CO emissions. Still, the emissions show similar qualitative trends with respect to the injection timing. The mechanism of Seiser always leads to a higher amount of CO for a specified sampling timing. Obviously the Seiser mechanism is slower (Figure 4(b)) and there is not enough time and oxygen for complete conversion to CO_2 especially in richer zones and this is why CO emissions go up. Furthermore, the mechanism of Andrae is more sensitive to injection timing than the rest of the two mechanisms.

All mechanisms have similar CA10 trends (identical sensitivity) with respect to the injection timing. Again there is a quantitative difference among them. This analysis indicates how emissions and combustion phasing results are sensitive to various mechanisms. It is not easy to determine the suitability of the mechanisms. Apparently the simulations with the mechanism of Seiser ignites too late for this application. Although the reduced Peters mechanism shows the best results, the more detailed Andrae mechanism is applied during the rest of the study since the mechanism has a broader applicability especially for more fuels.

4.3 Effect of inter-zonal mixing

Ignition delay and emissions levels are determined by the balance of chemical kinetics and the mixing event. There is no control over the evolution of the emissions for PCCI-like combustion as the combustion event is mainly governed by kinetics. In the XCCI code, inter-zonal mixing is included via the turbulent diffusivity factor. Typically it is possible to match CO emissions by tuning this diffusivity factor (C_t) for a specified case. To determine the magnitude of this factor the fuel-air mixing evolution for a non-reaction case is computed with the multi-zone model (XCCI) and compared to the actual evolution obtained from the CFD simulation. In Figure 5, fuel mass fractions are given as a function of zone number. Letters A, B and C refer to the moments at 13, 18 and 23^{o}CA aEOI, respectively. The fuel-air mixing becomes comparable to that of the CFD model with the turbulent diffusivity (C_t=8000). There is still a deviation, especially for the richest zone. This is mainly explained by the fuel penetration into crevices, which avoids proper mixing in this region for the CFD model. This effect is not captured currently in the multi-zone approach.

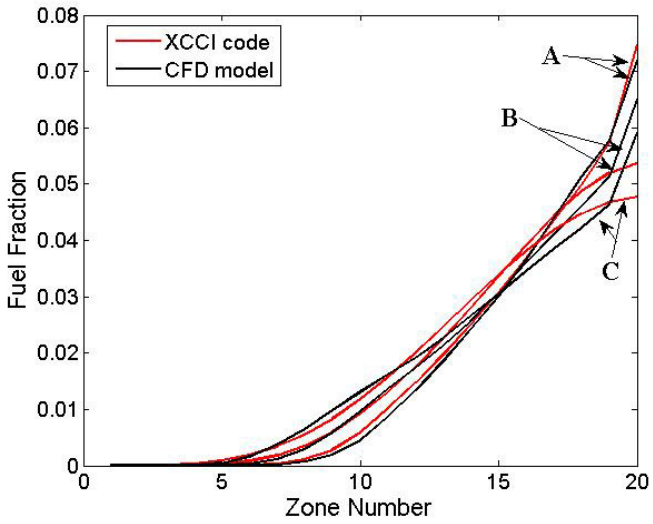

Fig. 5: Comparison of the fuel stratification between XCCI code with mixing (red lines) and CFD (black lines) model. XCCI simulation is initialized at SOI = 50°CA bTDC (C_t=8000).

A sensitivity analysis is performed with respect to C_t (C_t:1, 100, 500, 1000 and 2000) for two injection timings (SOI: 35 and 50°CA bTDC). The sampling moment for stratification is chosen as 13°CA aEOI and the heat loss to the cylinder walls is taken into account.

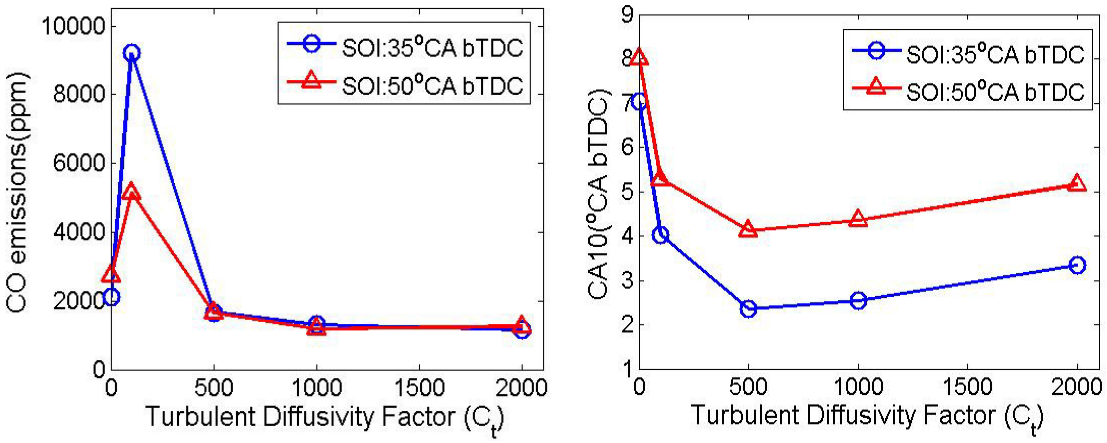

Fig. 6 (a) CO emissions (b) CA10 as a function of turbulent diffusivity factor.

Figure 6(a) displays that CO emissions are higher for the low mixing case (C_t=100) compared to the no mixing case. This is combined with an abundant amount of UHC emissions. When there is no mixing, the combination of the rich mixture and the heat loss to the cylinder walls creates zones which fail to ignite leading to excessive amount of UHC emissions (>10000ppm). Even with a small amount of mixing, UHC emissions are reduced drastically (to ~250ppm) whilst there is a huge rise in CO emissions (Figure 6(a)) due to incomplete combustion. The CO emissions become insensitive to the magnitude of mixing after C_t=1000. Therefore, C_t=1000 can be set as a reasonable approximation based on this analysis to represent the high level of mixing. C_t=100 is selected as the second turbulent diffusivity factor in order to investigate the influence of different mixing levels.

The mixing event retards ignition by decreasing the reactivity of the most reactive zones until a certain degree of mixing. After C_t=500, combustion is advanced slightly.

Still the difference between C_t=500 and 2000 is smaller than 1°CA for both injection timings.

4.4 Effect of stratification levels

In this final subsection, the effect of fuel distribution/stratification used as the initial condition for the injection model is studied. The sampling moments that are used to determine the initial charge stratification are defined with respect to the end of injection (See Figure 7) of the particular case under study (defined by its experimental SOI). The initial condition is then determined according to the crank angles after the end of injection at which the fuel distribution from CFD is sampled.

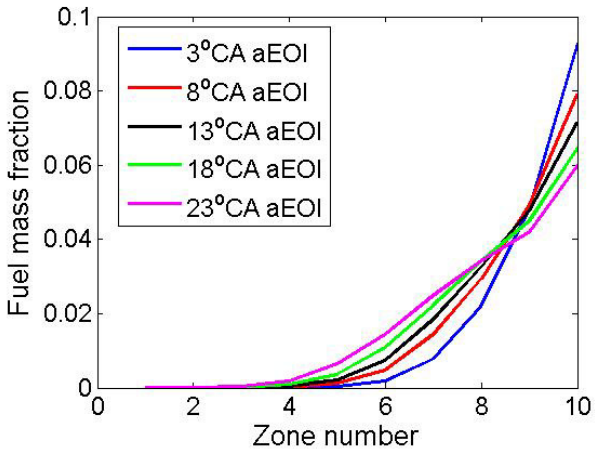

Fig. 7 Fuel distributions at various sampled timings (SOI: 35°CA bTDC).

Two injection timings are investigated with different stratification levels. Five different sampling moments (3, 8, 13, 18 and 23°CA aEOI) are chosen to analyze this

effect for the SOI: 35°CA bTDC case and four moments (3, 13, 23 and 33°CA aEOI) are used to define the SOI: 50°CA bTDC case. As expected, later sampling moments result in less stratified distributions. In addition to C_t=1000 (blue line), the simulations are repeated with C_t=100 (red line) to comprehend the effect of mixing on stratification in Figure 8.

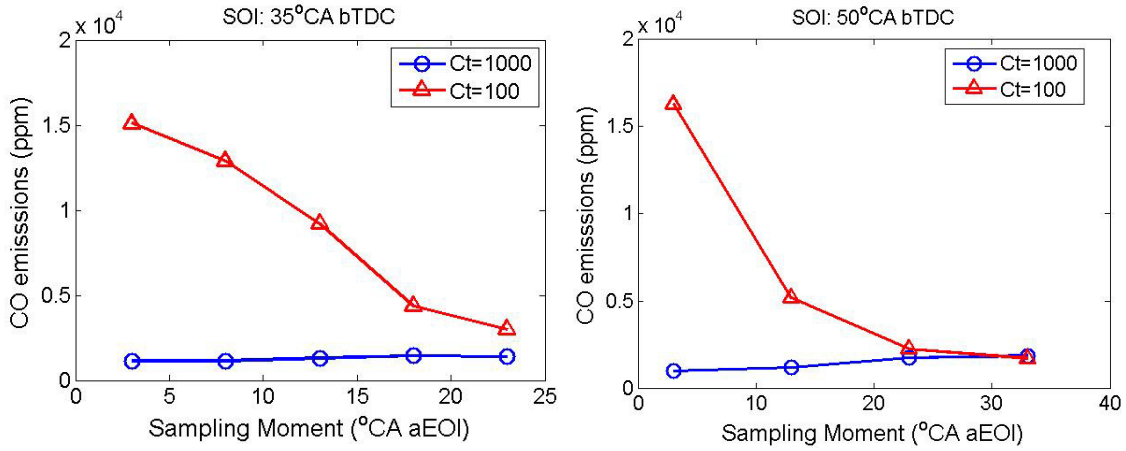

Fig. 8 The effect of stratification on CO emissions for SOI: (a) 35°CA and (b) 50°CA bTDC cases.

Figure 8 explains the motivation to set the turbulent diffusivity factor as C_t=1000. The effect of different stratification levels on CO emissions is clearly noticed for the low diffusivity constant (C_t=100). At later coupling moments more mixing has occurred in the CFD simulation and CO emissions are lowered due to the increased homogeneity. This dependence of the emissions on the sampling moment is decreased drastically with larger diffusivity. This is an important outcome since one of the sensitivity variables can be eliminated in this way. In other words, no matter which sampling moment is chosen

for a specified injection timing, similar results are obtained. It is now sufficient to choose one of the coupling moments as default.

When zonal mixing is introduced, O_2 diffuses from leaner zones to richer zones leading to an increase in combustion efficiency and CO consumption. For demonstration, the zonal CO emissions are presented in Figure 9 for the SOI: 40°CA bTDC case with sampling moment 13°CA aEOI. Zone 1 and 10 refer to the leanest and richest zones, respectively. The source of CO emissions is the relatively colder zones where the temperature is not sufficient to reach complete combustion albeit the values are negligible compared to low mixing cases. When there is very low mixing between the zones, the richer zones, where there is not enough O_2, are the main source of high CO emissions (Figure 9(b)). It is also found for some cases that the outer zone does not contribute to CO production due to the high heat loss to the cylinder walls and it becomes the major source for UHC emissions.

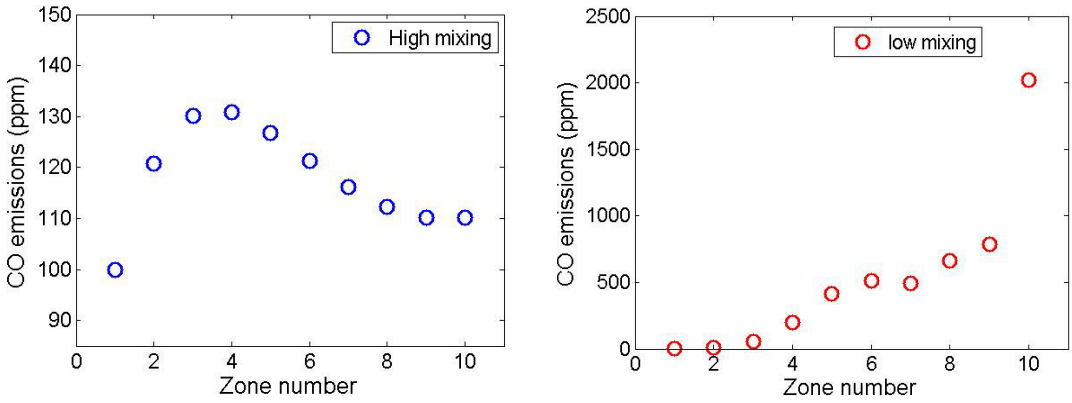

Fig. 9 CO emissions as a function of zone number (a) with high mixing (b) low mixing for SOI: 40°CA bTDC.

The final set of simulations is performed with respect to the injection timing. Note that choosing an arbitrary sampling moment is adequate based on the stratification analysis. Still more homogeneous distributions prior to ignition are expected for earlier injection timings, in accordance with that coupling at 10°CA bTDC is applied for all injection timings. In other words, the sampling moment of 10°CA bTDC corresponds to 8 and 33°CA bTDC for SOI: 25° and 50°CA bTDC cases, respectively which means obviously a more homogenous distribution for the latter one.

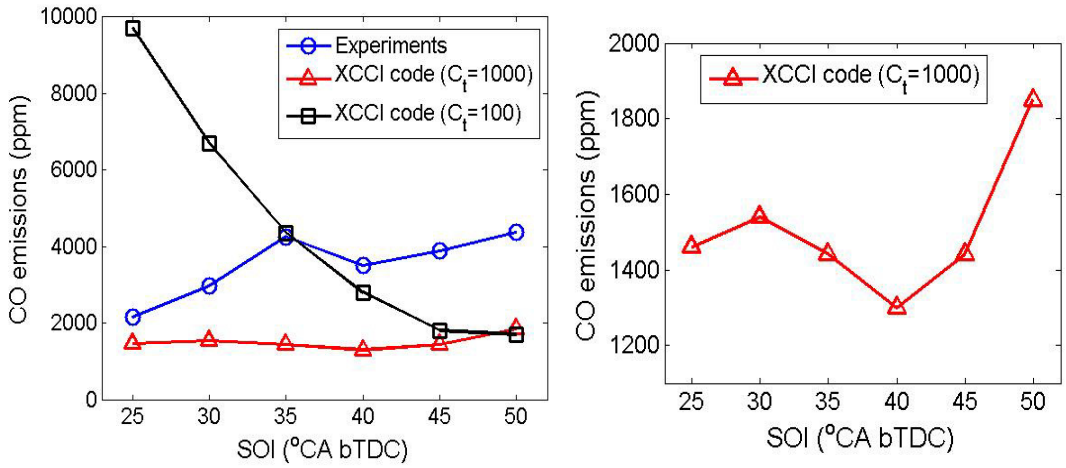

Fig. 10 CO emissions as a function of injection timing for experiments (blue), XCCI code with high mixing, C_t=1000 (red) and XCCI code with low mixing, C_t=100 (black). The right figure is a zoom of the results with C_t=1000.

It is observed in Figure 10 that CO emissions are under-predicted compared to the experimental values when intensifying the zonal mixing. Yet the trend is significantly

improved and the deviation is reduced. Several reasons can be listed to explain the quantitative deviation from the experiments. First of all, the difference between actual and computed ignition delay will affect CO emissions which causes an uncertainty due to the reaction mechanisms. Furthermore, mixing is needed mainly to account for the post ignition dynamics. However, CO emissions in experiments might be due to local isolated zones (crevices) that either do not ignite at all (UHC emissions) or progress too slowly due to excessive cooling (CO emissions). Such an isolated location cannot be modeled in the current approach. The amount of fuel in these crevices really depends on injection timing.

Finally, the combustion phasing results are compared (Figure 11(a)). The qualitative trend of ignition timing is satisfactory. The ignition is retarded with stronger mixing as mentioned in section 4.3. As an illustration, the (logarithmic) pressure-volume diagram is plotted for SOI: 45^{o}CA bTDC. It is shown in Figure 11(b) that the compression slope of the simulated curve matches experimental results. The ignition occurs a little bit later in the XCCI code. Due to higher combustion efficiency (lower CO emissions) the pressure trace is slightly over-predicted during the expansion stroke.

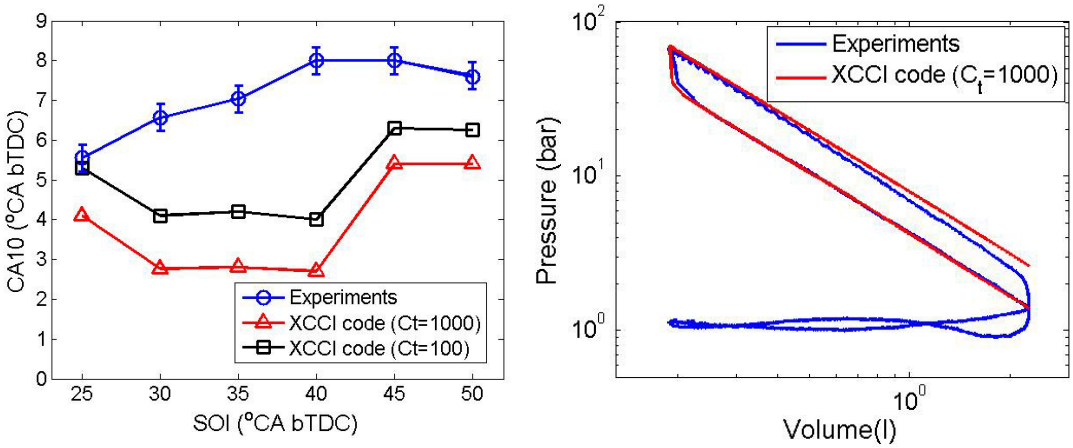

Fig. 11 (a) CA10 emissions as a function of SOI for experiments (blue), XCCI code with high mixing (red) and XCCI code with low mixing (black) (b) A logarithmic p-V diagram comparison between the XCCI code and the experiment for SOI: 45°CA bTDC.

5. Conclusions

A multi-zone model including inter-zonal mixing is used to analyze PCCI combustion while the results are compared with those of experiments. The main conclusions of this study are:

1. A totally homogeneous mixture in a single zone analysis avoids CO and UHC emissions in the model. 10 zones are sufficient to cover the zonal effects for emissions and combustion phasing analysis.

2. The reaction mechanisms show similar trends with respect to start of injection timing. The difference among the mechanisms indicates the difficulty to obtain a quantitative match with experimental results.

3. Including inter-zonal mixing is significant to improve the consistency and accuracy of the results. Different stratification levels have a drastic influence, especially on CO emissions when there is a low amount of mixing. This dependence can be significantly reduced with inter-zonal mixing where the turbulent diffusivity factor is determined from a sensitivity study.

The next step is to perform a study, which has a wider range of injection timing, with well-defined ignition trends. Besides, the stratification level can be determined by a simpler model instead of a CFD study. In this manner the computational efficiency can be increased further.

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Abbreviations

aEOI	After End of Injection
bTDC	Before Top Dead Center
CA	Crank Angle
CA10	Crank Angle which is defined as 10% of the total heat released
CFD	Computational Fluid Dynamics
CI	Compression Ignition
CO	Carbon Monoxide

CO_2	Carbon Dioxide
EGR	Exhaust Gas Recirculation
HCCI	Homogeneous Charge Compression Ignition
HD	Heavy Duty
IVC	Intake Valve Closing
LTC	Low Temperature Combustion
NO_x	Oxides of Nitrogen
PCCI	Premixed Charge Compression Ignition
ppm	Parts Per Million
PRF	Primary Reference Fuels
SI	Spark Ignition
SOI	Start of Injection
UHC	Unburned Hydrocarbons

Greek letters

λ	excess air ratio
φ	equivalence ratio

Symbols

c_v	heat capacity of the mixture
$c_{v,i}$	heat capacity of species i
D_z^i	symbolic representation of the diffusive mixing for the species.
D_z^T	turbulent diffusive mixing between the zones
e_i	internal energy of species *i*

h_i	enthalpy of species *i*
Mi	molecular weight of species *i*
M_z	zone average molecular weight
m_z	total zone mass
$m_{z,i}$	mass of species i
$\dot{m}_{z,i}^{in/out}$	mass flow through the boundaries
N_r	number of reactions
N_s	number of species
$\dot{Q}_z$	heat transfer rate due to heat loss and evaporative cooling during the fuel injection
p	pressure
R_u	universal gas constant
T_{in}	temperature of the intake flow
T_z	zone temperature
v_{ij}	stoichiometric coefficient of species *i* in reaction *j*
V_z	zone volume
Yi	mass fraction of species i
ω_j	reaction rate of reaction *j*

Subscripts

i	species
j	reaction
z	zone