Premixed charge compression ignition combustion modeling with a multi-zone approach including inter-zonal mixing

Citation for published version (APA):

Egüz, U., Leermakers, C. A. J., Somers, L. M. T., & Goey, de, L. P. H. (2013). Premixed charge compression ignition combustion modeling with a multi-zone approach including inter-zonal mixing. *Proceedings of the Institution of Mechanical Engineers. Part D : Journal of Automobile Engineering*, 227(9), 1313-1324. <https://doi.org/10.1177/0954407012474193>

DOI:

[10.1177/0954407012474193](https://doi.org/10.1177/0954407012474193)

Document status and date:

Published: 01/01/2013

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

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Proc IMechE Part D:
J Automobile Engineering
227(9) 1313–1324
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sagepub.co.uk/journalsPermissions.nav
DOI: 10.1177/0954407012474193
pid.sagepub.com

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Abstract

Premixed charge compression ignition combustion is a clean and efficient alternative to classical diesel combustion. The concept of premixed charge compression ignition combustion is associated with early injection of the fuel while applying high exhaust gas recirculation levels and operation with a highly lean mixture such that ignition takes place (well) after the injection event. Thus, it is possible to reduce the soot emissions and the nitrogen oxide emissions simultaneously. Premixed charge compression ignition combustion is analysed using a multi-zone model. In the multi-zone model, chemical mechanisms which are much more detailed than those used in the computational fluid dynamics approaches can be introduced directly. The computational fluid dynamics 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, basic inter-zonal diffusive mixing is applied. The level of mixing is estimated with a sensitivity study. When the inter-zonal mixing is included, the emission results become much less sensitive to the crank angle at which the charge stratification is sampled and the simulation is initialized.

Keywords

Premixed charge compression ignition, multi-zone modelling, stratification, detailed chemistry

Date received: 24 September 2012; accepted: 11 December 2012

Introduction

Since emission regulations have become more stringent, new combustion concepts should be developed to meet these emission standards. Although compression ignition (CI) engines lead to lower carbon dioxide (CO₂) emissions because they have a higher efficiency than spark ignition (SI) engines have, they suffer from high nitrogen oxide (NO_x) emissions and high 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 engines and the high efficiency of conventional CI engines.

PCCI combustion avoids circumstances which result in high NO_x and soot emissions.^{1–3} Very low NO_x emissions are achieved using this concept by operating with a highly diluted mixture which lowers the in-cylinder temperature, resulting in low-temperature

combustion. 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 the 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

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uncoupled from fuel injection, combustion timing control in the case of autoignition becomes a difficult issue in engine development and calibration. To decrease the development and calibration time and costs, the significance of numerical modelling increases even more.

As PCCI-like combustion is mainly governed by autoignition 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 modelling has been applied extensively in the engine community.⁸⁻¹⁶ In those studies, 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 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 markedly.

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. Also, a basic mixing model is applied in the multi-zone model (XCCI code²⁵). 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 later. 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 diesel engine using *n*-heptane as the fuel. This fuel has a cetane number that is comparable with 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 modelling 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 modelling approach is described including the XCCI-CFD interaction. Then, the experimental set-up is presented. In the results section, the effects of different modelling parameters, i.e. the number of zones, the chemical mechanisms, the inter-zonal mixing and the stratification level, are discussed.

Modelling approach

The XCCI code is a multi-zone code developed to perform PCCI and homogeneous charge compression ignition (HCCI) 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 neighbouring 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.

Mathematical model

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

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

where the subscripts z and i are used to denote the zone and the 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 respectively of species i . The 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. $\dot{m}_{z,i}^{in}$ and $\dot{m}_{z,i}^{out}$ are the mass flows 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 and is given by

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

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' , and λ is the laminar conduction coefficient.

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

The change in the 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) according to

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

The 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 and ω_j is the reaction rate of reaction j . Furthermore, v_{ij} is the stoichiometric coefficient of species i in reaction j . M3 is given by

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

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

$$pV_z = m_z \frac{R_u}{M_z} T_z \quad (5)$$

where R_u is the universal gas constant and M_z is the zone-averaged 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 according to

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

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.

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 Assanis²⁶ 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 from 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 the pressure p and for each zone the temperature, the volume and the mass of each species, namely V_z , T_z and $m_{z,i}$ respectively. 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. the differential-algebraic system solver (DASSL)²⁷).

Chemical model

Since the chemistry of commercially available fuels is not yet understood, surrogate fuels have received much attention lately. Surrogate fuels are based on primary reference fuels (PRFs), e.g. *n*-heptane and iso-octane (others also exist; see the paper by Farrell et al.²⁸), augmented with additional submechanisms (e.g. toluene) to model the fuel chemistry over a wider range of conditions.

In this paper, three chemical mechanisms are included. The first is the well-known semidetailed gasoline surrogate mechanism described by Andrae et al.²⁹ and based on a skeletal *n*-heptane or 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 reported by Seiser et al.³⁰ It is based on the detailed *n*-heptane mechanism described by Curran et al.³¹ (556 species and 2540 reactions) reduced systematically to 159 species and 770 reactions. The last mechanism (48 species and 248 reactions) is derived from the mechanism detailed by Peters et al.³² in which the C1–C3 submechanism replaces that of GRI3.0.³³

Initial conditions

The simulations are initialized at the moment of intake valve closing by setting the inlet temperature, the inlet pressure, the total cylinder mass and the mixture composition (calculated from the EGR level) from the experimental data. The initial conditions are the same for all zones. All zones have the same temperature, volume and mixture composition during the start of the simulation. The mixture composition differs between the zones owing 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-to-air ratio. It obviously cannot be measured in the full metal engine. Thus, the stratification level is obtained from the 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

Figure 1. Sample fuel mass fraction levels at different CAs (40° CA bTDC and 15° CA bTDC respectively) for an early-injection case (SOI, 50° CA bTDC; end of injection, 43° CA bTDC).

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

CA: crank angle; aEOI: after end of injection.

fuel distribution as a function of the injection timing. For illustration, the computed fuel contours for a start of injection (SOI) of 50° crank angle (CA) before top dead centre (bTDC) case are presented in Figure 1.

To determine the different levels of stratification in the multi-zone simulations the actual fuel distribution per simulated case is sampled at various CAs (Figure 2(a)). In this approach a direct mapping is applied at a sampling moment from three dimensions to one dimension 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 any longer. The results were quite similar. The reason for this is that the richest cells always exist near the cylinder wall, as illustrated in Figure 1. Irrespective of 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 carbon monoxide (CO) emissions and the details of the distribution do not play a major role.

The normalized fuel fraction for injection is defined on the basis of 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 by 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 the results are expected to depend. Thus, different sampling moments are chosen to perform a sensitivity study.

Experimental set-up and measurement series

Measurement programme

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 such as the EGR level, the intake temperature, the intake pressure and the injection timing.

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

Experimental engine set-up

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

Fed by an Atlas Copco air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. The non-firing cylinders 2 and 3 function as EGR pump cylinders, the purpose of which is to generate an adequate EGR flow, which is cooled both upstream and downstream of the pump cylinders.

Fuel to cylinder 1 is provided by a double-acting air-driven Resato HPU200-625-2 pump and an accumulator is placed near (about 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 eight holes of 0.151 mm diameter with a cone angle of 153°.

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 (TUE-DACS) and a SMETEC COMBI CA-resolved data acquisition system is used to record and process the cylinder pressure data. For more information on the experimental set-up and procedures, the

Table 1. CYCLOPS specifications.

Base engine	Six-cylinder heavy-duty direct-injection diesel
Cylinders	One, isolated for combustion
Bore (mm)	130
Stroke (mm)	158
Compression ratio	12:1
Bowl shape	M shaped
Bowl diameter (mm)	100

Table 2. Operating conditions.

Engine speed	1200 r/min
Fuel injection pressure	1500 bar
Fuel temperature	307 K
Intake air temperature	300 K
Injection durations	900 μ s, 1200 μ s, 1600 μ s
Intake pressure levels	1.25–1.5 bar
EGR levels	0 wt %, 15 wt %, 40 wt %, 50 wt %, 60 wt %

EGR: exhaust gas recirculation.

reader is referred to the papers by Leermakers et al.³⁵ and Boot et al.³⁶

Measurement matrix

For all experiments, a number of parameters are 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.

For every combination of operating conditions under investigation, a sweep of the start of actuations (SOA) of the injector is performed. Starting from conventional CI timings, the SOA is advanced at 5° increments, skipping SOAs at which combustion is not acceptable. Acceptable combustion in this aspect is defined by both the engine hardware limitations and the combustion quality targets.

Results

The main purpose of this study is to analyse the effects of the modelling parameters rather than the effects of the engine operating conditions. It is aimed to develop and present a predictive model together with its sensitivities to submodels. Thus, one operating point for each variable operating condition is chosen (the injection duration is 900 μ s, the intake pressure is 1.25 bar and the EGR level is 50%). The only difference between the studied cases is the SOI. The SOI is varied from 50° CA bTDC to 25° CA bTDC with 5° intervals. The numerical results will be analysed with respect to the combustion phasing and CO emissions. CO emissions are utilized especially to judge the significance of

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

SOI (deg CA bTDC)	Sampling moment (deg CA bTDC)	Nomenclature
30	5	D1
50	30	D2

SOI: start of injection; CA: crank angle; bTDC: before top dead centre.

inter-zonal mixing. First, the sensitivity of the results to the number of zones and the applied chemical mechanism will be determined. Then, with the optimal settings the effects of the inter-zonal mixing and, related to that, the degree of stratification are investigated.

Effect of the number of zones

The advantage of the multi-zone model compared with 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 one zone, five zones, 10 zones, 20 zones and 40 zones are compared. The chemical mechanism described by Andrae et al. 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 analyse the pure effect of the number of zones, the heat loss to cylinder walls and the zonal mixing are ignored here.

When the total CO emissions (Figure 3(a)) are compared, the effect of the 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 $\lambda \approx 2.4$) 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 arises because, for this setting, more fuel is injected in the outer zones where there is heat loss to the cylinder walls. Because of 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 hydrocarbon (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.

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 the start of combustion, which in turn can be utilized to indicate the combustion phasing. Here, the excess amount of oxygen 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 and from 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 the default for the rest of the study.

Effects of the 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 13° CA after the end of injection (aEOI) for the three different reaction mechanisms.

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

All mechanisms have similar CA10 trends (identical sensitivities) with respect to the injection timing. Again there is a quantitative difference between 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 Seiser et al. mechanism ignites too late for this application. Although the reduced Peters et al. mechanism shows the best results, the more detailed Andrae et al. mechanism is applied during the rest of the study since the mechanism has a broader applicability especially for more fuels.

Effect of the inter-zonal mixing

The 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, the 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 with the actual evolution obtained from the CFD simulation. In Figure 5, the fuel mass fractions are given as functions of the zone number. The letters A, B

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

CO: carbon monoxide; CA10: crank angle where 10% of the total heat is released; CA: crank angle; bTDC: before top dead centre.

Figure 4. (a) CO emissions and (b) CA10 as functions of the SOI for three different reaction mechanisms.

CO: carbon monoxide; SOI: start of injection; CA: crank angle; bTDC: before top dead centre. CA10: crank angle where 10% of the total heat is released.

and C refer to the moments at 13° CA aEOI, 18° CA aEOI and 23° CA aEOI respectively. The fuel–air mixing becomes comparable with 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.

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

Figure 6(a) demonstrates that the CO emissions are higher for the low-mixing case ($C_t = 100$) than for 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 (greater than 10,000 ppm). Even with a small amount of mixing, the UHC emissions are reduced drastically (to about 250 ppm) while there is a huge rise in the 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 a high level of mixing. $C_t = 100$ is selected as

Figure 5. Comparison of the fuel stratification between the XCCI code with mixing (red curves) and CFD (black curves) model. XCCI simulation is initialized when the SOI is at 50° CA bTDC ($C_t = 8000$). CFD: computational fluid dynamics.

the second turbulent diffusivity factor in order to investigate the influence of the 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 $C_t = 2000$ is smaller than 1° CA for both injection timings.

Effects of the stratification levels

In this final section, the effect of the fuel distribution or 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 (Figure 7) of the particular case under study (defined by its experimental SOI). The initial condition is then determined according to the CAs aEOI at which the fuel distribution from CFD is sampled.

Two injection timings are investigated with different stratification levels. Five different sampling moments (3° CA aEOI, 8° CA aEOI, 13° CA aEOI, 18° CA aEOI and 23° CA aEOI respectively) are chosen to analyse this effect for the case with the SOI at 35° CA bTDC, and four moments (3° CA aEOI, 13° CA aEOI, 23° CA aEOI and 33° CA aEOI respectively) are used to define the case with the SOI at 50° CA bTDC. As expected, later sampling moments result in less stratified distributions. In addition to $C_t = 1000$ (line with open circles), the simulations are repeated with $C_t = 100$ (line with open triangles) to comprehend the effect of mixing on stratification in Figure 8.

Figure 8 explains the motivation to set the turbulent diffusivity factor as $C_t = 1000$. The effect of the different stratification levels on the 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 owing to the increased homogeneity. This dependence of the emissions on the sampling moment is decreased drastically with higher diffusivity. This is an important outcome since one of the sensitivity variables can be eliminated in this way. In other words, irrespective of 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 the default.

When zonal mixing is introduced, O_2 diffuses from leaner zones to richer zones, leading to increases in the combustion efficiency and the CO consumption. As a

Figure 6. (a) CO emissions and (b) CA10 as functions of the turbulent diffusivity factor.

CO: carbon monoxide; SOI: start of injection; CA: crank angle; bTDC: before top dead centre. CA10: crank angle where 10% of the total heat is released.

Figure 7. Fuel distributions at various sampled timings (SOI, 35° CA bTDC).

CA: crank angle; aEOI: after the end of injection.

demonstration, the zonal CO emissions are presented in Figure 9 for the case with the SOI at 40° CA bTDC with a sampling moment of 13° CA aEOI. Zone 1 and zone 10 refer to the leanest zone and the richest zone 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 with the low-mixing cases. When there is very low mixing between the zones, the richer zones, where there is not sufficient oxygen, 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 owing to the high heat loss to the cylinder walls, and it becomes the major source for UHC emissions.

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 the fact 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° CA bTDC and 33° CA bTDC for the cases with the SOI at 25° CA bTDC and 50° CA bTDC respectively, which means obviously a more homogeneous distribution for the latter case.

It is observed in Figure 10 that the CO emissions are underpredicted compared with 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 the actual ignition delay and the computed ignition delay will affect the CO emissions, which causes an uncertainty due to the reaction mechanisms. Furthermore, mixing is needed mainly to account for the post-ignition dynamics. However, the CO emissions in the experiments might be due to local isolated zones (crevices) that either do not ignite at all (the UHC emissions) or progress too slowly because of excessive cooling (the CO emissions). Such an isolated location cannot be modelled in the current approach. The amount of fuel in these crevices really depends on the injection timing.

Finally, the combustion phasing results are compared (Figure 11(a)). The qualitative trend of the ignition timing is satisfactory. The ignition is retarded with stronger mixing as mentioned in the section on the effect of the inter-zonal mixing. As an illustration, the (logarithmic) pressure–volume diagram is plotted with the SOI at 45° CA bTDC. It is shown in Figure 11(b) that the compression slope of the simulated curve matches the experimental results. The ignition occurs slightly later in the XCCI code. Because of the higher combustion efficiency (lower CO emissions) the pressure trace is slightly overpredicted during the expansion stroke.

Figure 8. The effect of stratification on the CO emissions for the cases when the SOI is at (a) 35° CA bTDC and (b) 50° CA bTDC. CO: carbon monoxide; SOI: start of injection; CA: crank angle; bTDC: before top dead centre; aEOI: after the end of injection.

Figure 9. CO emissions as a function of the zone number (a) with high mixing and (b) with low mixing with the SOI at 40° CA bTDC. CO: carbon monoxide.

Figure 10. (a) CO emissions as a function of the injection timing for experiments (open circles), XCCI code with high mixing, $C_t = 1000$ (open triangles), and XCCI code with low mixing, $C_t = 100$ (open squares). (b) A zoom of the results with $C_t = 1000$. CO: carbon monoxide; SOI: start of injection; CA: crank angle; bTDC: before top dead centre.

Figure 11. (a) CA10 emissions as a function of the SOI for experiments (open circles with vertical bars), XCCI code with high mixing (open triangles) and XCCI code with low mixing (open squares). (b) A logarithmic p - V diagram comparison between the XCCI code and the experiment with the SOI at 45° CA bTDC.

CA10: crank angle where 10% of the total heat is released; CA: crank angle; bTDC: before top dead centre; SOI: start of injection.

Conclusions

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

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 the emissions and combustion phasing analysis.
2. The reaction mechanisms show similar trends with respect to the SOI timing. The difference between the mechanisms indicates the difficulty in obtaining a quantitative match with the experimental results.
3. Including inter-zonal mixing is significant in improving the consistency and accuracy of the results. Different stratification levels have a drastic influence, especially on the 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 timings, with well-defined ignition trends. Also, 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.

Funding

This work was supported by the Stichting voor de Technische Wetenschappen, which is the applied science division of the Nederlandse Organisatie voor Wetenschappelijk Onderzoek, and the technology programme of the Ministerie van Economische Zaken, Landbouw en Innovatie (Project number 10417).

Acknowledgements

DAF Trucks N.V., Shell Global Solutions, Avantium Chemicals B.V. and Delphi are also acknowledged for their contributions to the project.

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e_i
h_i
m_z
$m_{z,i}$
$\dot{m}_{z,i}^{in}, \dot{m}_{z,i}^{out}$
M_i
M_z
N_r
N_s
P
$\dot{Q}_z$

R_u
T_{in}
T_z
v_{ij}

V_z
Y_i

λ
ω_j | internal energy of species <i>i</i>
enthalpy of species <i>i</i>
total zone mass
mass of species <i>i</i>
mass flows through the boundaries
molecular weight of species <i>i</i>
zone-averaged molecular weight
number of reactions
number of species
pressure
heat transfer rate due to the heat loss and evaporative cooling during the fuel injection
universal gas constant
temperature of the intake flow
zone temperature
stoichiometric coefficient of species <i>i</i> in reaction <i>j</i>
zone volume
mass fraction of species <i>i</i>

excess air ratio
reaction rate of reaction <i>j</i> |
|--|---|
-
- Subscripts**
i
j
z | species
reaction
zone |
|-------------------|-----------------------------|
-
- Abbreviations**
aEOI
bTDC
CA
CA10

CFD
CI
CO
CO ₂
EGR
HCCI

NO _x
PCCI
PRF
SI
SOI
UHC | after end of injection
before top dead centre
crank angle
crank angle where 10% of the total heat is released
computational fluid dynamics
compression ignition
carbon monoxide
carbon dioxide
exhaust gas recirculation
homogeneous charge compression ignition
nitrogen oxides
premixed charge compression ignition
primary reference fuel
spark ignition
start of injection
unburned hydrocarbon |
|---|--|

Appendix I

Notation

c_v	heat capacity of the mixture
$c_{v,i}$	heat capacity of species <i>i</i>