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HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINE: A SIMULATION STUDY ON THE EFFECTS OF INHOMOGENEITIES

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ABSTRACT

A new stochastic model for the HCCI engine is presented. The model is based on the PaSPFR-IEM model and accounts for inhomogeneities in the combustion chamber while including a detailed chemical model for natural gas combustion consisting of 53 chemical species and 590 elementary chemical reactions. With this model the effect of temperature differences caused by the thermal boundary layer and crevices in the cylinder for a particular engine speed and fuel to air ratio is studied. The boundary layer is divided into a laminar film layer and a turbulent buffer zone. There are also colder zones due to crevices. All zones are modeled by a characteristic temperature distribution. The simulation results are compared with experiments and a previous numerical study employing a PFR model. In all cases the PaSPFR-IEM model leads to a better agreement between simulations and experiment for temperature and pressure.

In addition a sensitivity study on the effect of different intensities of turbulent mixing in the combustion is performed. This study reveals that the ignition delay is a function of turbulent mixing of the hot bulk and the colder boundary layer.

INTRODUCTION

The Homogeneous Charge Compression Ignition (HCCI) engine is a promising alternative to the existing Spark Ignition (SI) engines and Compression Ignition (CI) engines.

As in a diesel engine, the fuel is exposed to sufficiently high temperature for autoignition to occur, but for HCCI a homogeneous fuel/air mixture is used. The homogeneous mixture is created in the intake system as in a SI engine, using a low-pressure injection system or by direct injection with very early injection timing.

To limit the rate of combustion, very diluted mixtures have to be used. Compared to the diesel engines the HCCI has a nearly homogeneous charge and virtually no problems with soot and NOx formation. On the other hand HC and CO levels are higher than in conventional SI engines. Overall, the HCCI engine shows high efficiency and fewer emissions than conventional internal combustion engines.

The efficiency of the HCCI engine has previously been shown by a number of experiments. Parts of the experiments have been complemented by numerical studies modeling the engine as a plug flow reactor (PFR) [1][2]. In these simulations the ignition delay times for a set of different parameters were investigated. The results indicate that local inhomogeneities are responsible for differences between measurements and simulation results.

One way of accounting for these inhomogeneities is to use multiple zones to model boundary layer effects. Such work has recently been performed using a 10 zone-model for the HCCI engine [12]. Another way is to use a model that is based on the probability density function of the physical variables that are important in the combustion process. If one wishes to study chemical reactions in detail, simplifying assumptions have to be introduced because the numerical cost to solve a model that describes chemistry and all aspects of flow would be too high.

One way to reduce this cost is to assume that chemical species and temperature are random variables with a Probability Density Function (PDF) that does not spatially vary in the combustion chamber i.e. temperature and composition can fluctuate. This assumption is not as strong as the assumption made in case of the PFR model where the physical quantities are not random variables and they are homogeneous all over the combustion chamber.

The **purpose of this paper** is to introduce a new simulation model featuring the partially stirred plug flow reactor (PaSPFR) as described in refs. [3][4]. Numerical simulations of the ignition process in the HCCI engine will be performed using a detailed chemical model for butane and lower alkanes in the framework of the PaSPFR. The reaction mechanism contains 53 chemical species and 590 elementary chemical reactions. In the PaSPFR model the unclosed term for turbulent micromixing has been modeled by the simple deterministic IEM mixing model.

The PaSPFR model will be used in an attempt to improve on previous numerical simulations of the HCCI process taking fluctuations in temperature that are induced by the colder thermal boundary layer into account. The results of the new PDF based model and the old PFR model are compared to the experiment in ref [1]. Additionally, we perform a sensitivity study on the influence of turbulent mixing on ignition delay. The effect of different mixing intensities on the mean of temperature and pressure as well as their standard deviation (STD-DEV) will be discussed.

NOMENCLATURE

Abbreviations

HCCI	: Homogeneous Charged Compression Ignition
PFR	: Plug Flow Reactor
PaSPFR	: Partially stirred Plug Flow Reactor
PDF	: Probability Density Function
MDF	: Mass Density Function
IEM	: Interaction by Exchange with the Mean mixing model
STD-DEV	: Standard Deviation
ATDC	: After Top Dead Center
BTDC	: Before Top Dead Center
BBTC	: Before Bottom Dead Center
CAD	: Crank Angle Degree
CR	: Compression ratio
RPM	: Revolutions per minute

Arabic symbols

a	: Crank radius
A	: Cylinder surface area
B	: Bore
C_v	: Specific heat at constant volume
C_ϕ	: Proportionality constant
F_ϕ	: Joint scalar mass density function
h_i	: Specific enthalpy of species *i*
l	: Connecting rod
l_i	: Integral length scale
M_i	: Molecular weight of species *i*
M	: Mean molecular weight
m	: Mass
p	: Pressure
T	: Temperature
t	: Time
Q_i	: Source term
R	: Universal gas constant
R_x	: Autocorrelation coefficient
V	: Volume
V_c	: Compression volume
$w^{(n)}$	: Mass weight for PDF
Y_i	: Mass fraction of species *i*

Greek Symbols

α	: Heat transfer coefficient
$\hat{\varepsilon}$	: Emissivity
ε	: Dissipation
ϕ	: Equivalence ratio
$\underline{\phi}$	: Joint scalar random vector
Θ	: CAD
ν_{ij}	: Stoichiometric coefficients
ρ	: Density
τ	: Turbulent velocity time scale
τ_ϕ	: Turbulent scalar time scale
$\underline{\psi}$	: Joint scalar sample variable
ω_j	: Rate of reaction *j*

Sub- and Superscripts

BL	: Index for boundary layer
Bulk	: Index for bulk
I	: Index for scalars
J	: Index for reactions
n	: Index for scalar state
S	: Number of chemical species
R	: Number of reactions
w	: Wall

PREVIOUS MODEL AND EXPERIMENTAL RESULTS

The experimental results used in this work are the same as those described in [1].The experimental setup is as follows :

A six-cylinder Volvo TD100 series truck diesel is used, modified for one-cylinder use, and converted to HCCI operation. The engine data are given in Table 1, additional details can be found in [1] and [2]. The simplest possible combustion chamber geometry is used, i. e. a flat piston crown giving a pancake combustion chamber.

Common commercially available natural gas is used as fuel [2]. The predominate compound of the natural gas is methane, with a non-negligible content of other gases, mainly higher hydrocarbons such as ethane, propane and butane (see Table 2 for details).

Table 1 : *Volvo TD100 engine parameters.*

Displaced Volume	1600 cm^3
Bore	120.65 mm
Crank radius	70 mm
Stroke	140 mm
Connection Rod	260 mm
Exhaust Valve Open	39° BBDC (at 1 mm lift)
Exhaust Valve Close	10° BTDC (at 1 mm lift)
Inlet Valve Open	5° ATDC (at 1 mm lift)
Inlet Valve Close	13° ABDC (at 1 mm lift)

Table 2 : *Natural gas components***.**

Component	Mole-%	Mass-%
Methane	91.3	81.0
Ethane	5.0	7.9
Propane	1.8	4.2
n-Butane + higher	1.0	4.7
Nitrogen	0.3	0.9
Carbon dioxide	0.6	1.2

The engine is run on natural gas at fuel-air ratios of ϕ = 0.30–0.45. Four different engine speeds are used: 800, 1000, 1200 and 1400 rpm. These engine speeds are chosen as being representative for normal use considering that maximum torque for a normal CI-operating TD100-series diesel is achieved at 1400 rpm and the engine idle speed is 475–525 rpm. In this work we will focus on the operating conditions stated in Table 3, measured at 60 CAD BTDC.

The fact that the fuel and oxidizer is assumed to be perfectly mixed gives a very steep increase in temperature upon ignition. In reality not all of the mixture will reach ignition conditions at exactly the same time, which results in a less steep ignition curve as seen in the experimental results in Figure 1.

Table 3: *Initial values for the simulations of engine case (60 CAD BTDC).*

ϕ	CR	T [K]	P [BAR]	RPM
0.368	17.30	664	4.40	1000

The previous numerical studies model the HCCI engine as a simple PFR and thus ignore influences of local inhomogeneities in the cylinder. An example of results from the previous work can be seen in Figure 1 in ref. [1].

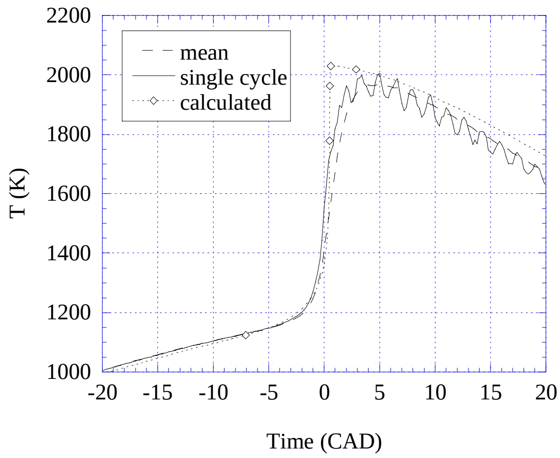

Figure 1: *Numerical results from the PFR model compared with experiments. The TD100 engine is in this case run at 1000 rpm and ϕ = 0.368. The jagged line represents results from a single experimental engine cycle and the broken line is its smoothed version.*

Because of the use of a detailed reaction mechanism in the PFR model the ignition timing is however predicted correctly.

The oscillations in the single cycle curve are due to pressure oscillations. The temperature is evaluated directly from the pressure. The origin of the pressure oscillations is not fully understood. Most likely the rate of combustion is so fast that the pressure gradient in the cylinder generates vibrations in the engine structure. These then result in volume changes in the cylinder and hence pressure oscillations [private communication with B. Johansson].

MODELING THE BOUNDARY LAYER

As stated above the assumption of homogeneity is responsible for a too high temperature rise rate during ignition. To overcome this assumption we model instead the existence of a colder boundary layer of gas near the cylinder wall.

The thickness of this boundary layer has recently been investigated experimentally on the TD100 series engine [7]. These experiments suggest that the thickness of the boundary layer is approximately 3 millimeters. The same result can be obtained from Heywood [8] for the general case. For the current HCCI engine setup a boundary layer of 3 mm corresponds to approximately 10 % of the displaced cylinder volume. Since the boundary layer is assumed to be significantly cooler than the bulk gasses the total gas mass in the boundary layer will more likely be 15-20 %. Additionally we have to account for colder fluid parcels in crevices.

The boundary layer can be described by applying theories for the flow of a fluid passing a solid surface. It is therefore assumed to consist of a thin film layer immediately adjacent to the cylinder wall plus a “buffer zone” between this and the turbulent bulk flow [9]. The crevices are represented by the first five particles and the film layer corresponds to particle numbers 6 to 15 as illustrated in Figure 2. Within the film layer we have a strong increase in temperature. This is reflected by the large variance of temperature of the film layer particles. In the laminar zone heat is transferred primarily through conduction.

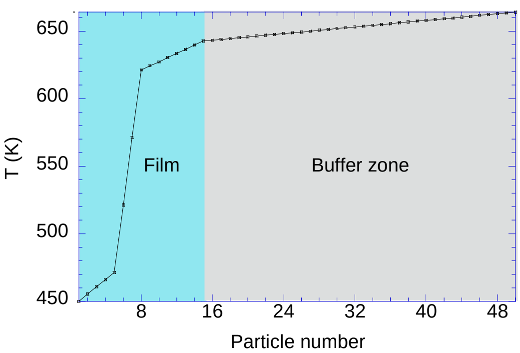

Figure 2: *Temperature distribution in the boundary layer. The temperature increases from the wall temperature and asymptotically approaches the bulk gas temperature.*

As one approaches the bulk of the cylinder the temperature increases asymptotically towards the bulk gas temperature (illustrated by the “Buffer zone” in Figure 2). In the figure above the wall temperature is 450K and the hot bulk gas is 650K. The boundary layer is modeled using 50 fluid particles representing the 3mm radius adjacent to the cylinder wall.

TURBULENT PHENOMENA IN THE ENGINE

Experimental results performed on the Volvo TD100 series engine give a quantitative description of the turbulent behavior of the gases in the cylinder [11]. These experiments have been performed when the engine is run in lean SI mode and for the inert case. In the following we will assume that the turbulence characteristics for the HCCI engine are comparable to these results. This assumption can be justified by the fact that the same pancake shaped combustion chamber is used in the two setups and that there is no influence on the flow from a propagating flame front in the experimental inert case.

The fluctuating velocity component is defined by the turbulence intensity u' as

$$u' = \lim_{t\to\infty}\left(\frac{1}{t}\int_{t_0}^{t_0+t} u^2 dt\right)^{½}$$

and the integral length scale l_I is defined as

$$l_I = \int_0^{\infty} R_x dx$$

where R_x is the autocorrelation coefficient of the fluctuating velocity.
The turbulence mixing time scale is in this case defined as the relation between the integral length scale and the fluctuating velocity component

$$\tau_\phi = \frac{\tau}{C_\phi} = \frac{1}{C_\phi}\frac{l_I}{u'}$$

where C_ϕ is a model constant.
The turbulent energy dissipation rate ε is given by

$$\varepsilon = \frac{(u')^3}{l_I}\ .$$

Measurements of turbulence intensity in the cylinder show fluctuations in the range of 0.5-0.9 m/s from 20 CAD BTCD to 20 CAD ATDC. The integral length scale is in the range of 10-18 mm. This gives turbulence mixing time scale in the order of 0.01s and a dissipation rate in the order of 10 m^2/s^3.

THE STOCHASTIC REACTORMODEL

In order to account for the inhomogeneities in the combustion chamber we use a stochastic reactor model PaSPFR-IEM as described in [3]. The assumption of homogeneity for species mass fractions and temperature that has been made previously in [1] is replaced by the assumption of statistical homogeneity. This means that the joint scalar PDF does not vary within the combustion chamber.

In the following we distinguish between global and local quantities. Global quantities are mass *m*, volume *V(t)*, mean density $\langle\rho(t)\rangle$ and pressure *p(t)*. We assume that global quantities do not vary spatially in the combustion chamber. Local quantities are chemical species mass fractions $Y_i(t)$,

i=1,...,S and temperature $T(t)$. They can vary within the combustion chamber and are assumed to be random variables. Their joint random vector is defined as

$$\underline{\Phi}(t) = (\Phi_1,...,\Phi_{S+1}) = (Y_1,...,Y_S,T)$$

and the corresponding joint scalar mass density function (MDF) is given by $F_{\underline{\Phi}}(\Psi_1,...,\Psi_{S+1};t)$ assuming spatial homogeneity as proposed in the PaSPFR model. Its time evolution is given by the following MDF-transport equation

$$\frac{\partial}{\partial t}F_{\underline{\Phi}}(\underline{\Psi};t) + \frac{\partial}{\partial \Psi_i}(Q_i(\underline{\Psi})F_{\underline{\Phi}}(\underline{\Psi};t)) = \frac{\partial}{\partial \Psi_i}(\frac{1}{2}\frac{C_\Phi}{\tau}(\Psi_i - \langle\Phi_i\rangle)F_{\underline{\Phi}}(\underline{\Psi};t))$$

where the initial conditions are given as $F_\Phi(\underline{\Psi};0) = F_0(\underline{\Psi})$. The brackets $\langle.\rangle$ denote the mean according to F_ϕ and C_ϕ/τ is a measure for the intensity of scalar mixing. The model constant C_ϕ is set to 2.0 and the turbulent time scale is estimated from the experiment as mentioned above. The right hand side of this equation describes the mixing of the scalars due to turbulent diffusion. This model is called IEM model and is known to have some deficiencies but due to its simplicity and low numerical cost it has been applied (details in Ref. [3]). The term Q_i describes the change of the MDF due to chemical reactions, change in volume, and heat losses.

$$Q_i = \frac{M_i}{\rho}\sum_{j=1}^{R}\nu_{i,j}\omega_j \qquad i = 1,...,S$$

$$Q_{S+1} = \frac{1}{c_v}\sum_{i=1}^{S}(h_i - \frac{RT}{M_i})\frac{M_i}{\rho}\sum_{j=1}^{R}\nu_{i,j}\omega_j + p\frac{1}{c_v}\frac{dV}{dt} - \frac{1}{c_v}(\alpha A(T - T_w) + A\sigma\hat{\varepsilon}(T^4 - T_W^4))$$

The convective heat transfer coefficient is obtained from the Woschni equation [8], σ is the Stefan-Boltzmann constant and the emissivity $\hat{\varepsilon}$ of methane [10] is used. Besides the MDF equation the time evolution of the global quantities has to be computed. The change of volume $V(\Theta(t))$ in terms of CAD is given by

$$V(\Theta(t)) = V_c + \frac{\pi \cdot B^2}{4}\left(l + a - a\cdot\cos(l^2 - a^2\cdot\sin^2\Theta(t))^{1/2}\right)$$

as in [8]. Mean density can be calculated as

$$\langle\rho(t)\rangle = \frac{m}{V(t)},$$

pressure is given by the ideal gas law

$$p(t) = \langle\rho(t)\rangle\frac{R\langle T\rangle}{\langle M\rangle}$$

where $\langle T\rangle$ is the mean temperature according to the MDF and $\langle M\rangle$ is the expected mean molecular weight. These equations as well as the transport equation of the MDF have to be solved simultaneously. For this work the stochastic reactor model is implemented into the existing code for HCCI engine calculations as described in [5][6]. The solution procedure is based on a stochastically weighted particle method and a higher order operator splitting technique. Details of the numerical procedure will be published separately.

INTIAL CONDITIONS

The simulations for the auto-ignition process were made using initial values obtained from the experiments at 60 CAD BTDC described in Table 3. The species composition in the boundary layer and the bulk is assumed to be identical. The only scalar variable that varies is temperature. The initial MDF is given by

$$F_0(\underline{\Psi}) = \underbrace{\sum_{n=1}^{BL} w^{(n)}\delta(\underline{\Psi} - \underline{\Psi}^{(n)})}_{BoundaryLayer} + \underbrace{w^{(BL+1)}\delta(\underline{\Psi} - \underline{\Psi}^{(BL+1)})}_{Bulk}.$$

The weights $w^{(n)}$ are chosen to be

$$w^{(n)} = \begin{cases} \frac{m_{BL}}{BL} & : \quad n = 1,...,BL \\ m_{B\,ulk} & : \quad n = BL + 1 \end{cases}$$

with $m = m_{BL} + m_{bulk}$ being the mass of the fuel-air mixture in the combustion chamber. m_{BL} is the mass of fuel-air mixture in the boundary layer and m_{bulk} is the bulk. The scalars $\Psi_j^{(n)}$ for j=1,...,S are the chemical species mass fractions and are all set to the same value to meet the conditions in Table 3. The temperature in the boundary layer $\Psi_{S+1}^{(n)}$: $n = 1,...,BL$ is set according to the temperature profile displayed in Figure 2. The temperature in the bulk $\Psi_{S+1}^{(n)}$: $n = BL + 1$ is set to a value to match the initial mean temperature in the combustion chamber. For the present case we model the boundary layer by choosing a turbulent mixing time scale (τ) of 0.02s and 20 % of the total gas mass in the boundary layer.

RESULTS AND DISCUSSION

In the following section we will demonstrate the capabilities of the new model and compare numerical results from this model to experimental results and results from the previous model described in [1]. In this case the engine is operating at 1000 rpm with a fuel to air ratio of 0.368. This is the case described in Table 3.

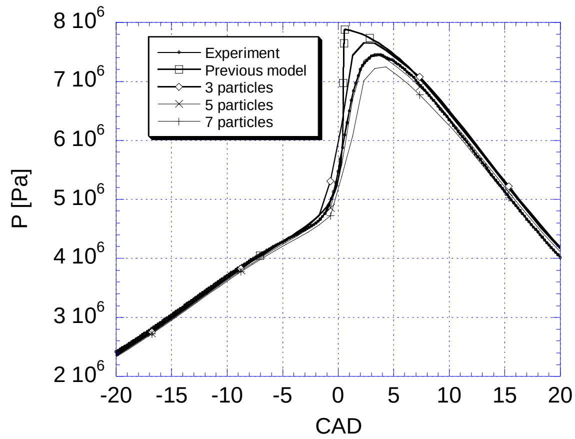

Figure 3: *Pressure history. New model compared to experimental results and previous model.*

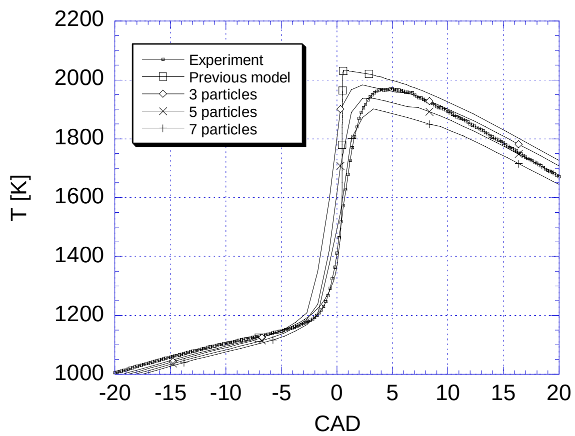

Figure 4: *Temperature history. New model compared to experimental results and previous model.*

Figure 3 illustrates the pressure history for this case. The number of fluid particles representing the laminar part of the film layer and the crevices is varied from 3 to 7. The shape of the ignition curve is independent of the number of cold particles in this part of the film layer but ignition timing and maximum pressure is affected. Choosing 5 fluid particles gives a simulated result nearly identical to the experimental results. The new model generally produces results significantly closer to the experiments than the previous model.

Figure 4 shows the temperature history for the same case. The experimental temperature history is not directly measured but calculated from the pressure measurements using a very simple 1-zone model. Therefore the simulated temperature is not directly comparable to the experimental results in this figure.

Figure 5 illustrates the standard deviation (STD-DEV) of the calculated temperature for the simulation. Again the number of fluid particles representing the laminar part of the film layer is varied from 3 to 7. The STD-DEV is slowly decreasing during the first inert part of the compression stroke due to the temperature mixing of fluid parcels in the bulk and in the boundary layer. At around 3 CAD BTDC the bulk ignites which leads to a rapid increase of

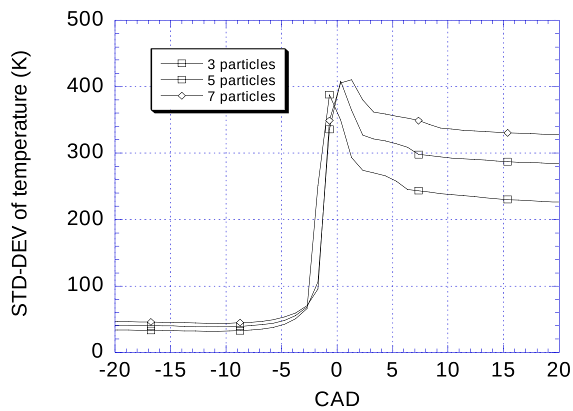

Figure 5: *STD-DEV of temperature history.*

STD-DEV. While the ignition process is progressing the STD-DEV decreases until most of the boundary layer has ignited. The difference in STD-DEV between the time before ignition and after ignition indicates that not all parts of the boundary layer are fully burnt.

Generally one can conclude from these first results that the implementation of the SRM greatly improves the numerical simulation of the HCCI process. The IEM mixing model does describes mixing adequately if the initial distribution of particles in crevices and boundary layer is sufficiently good. In the following sections 5 fluid particles are chosen to represent the laminar part of the film layer.

SENSITIVITY STUDY

In this section a sensitivity study on the new model will be presented. It will study the effects of varying the turbulence time scale (τ).

In Figure 6 the turbulence mixing time scale is varied from 0.1s to 0.0001s. The result of this study shows that a very slow mixing (τ=0.1s) will promote a very early ignition of the hot spots in the cylinder since they do not mix with the cold spots.

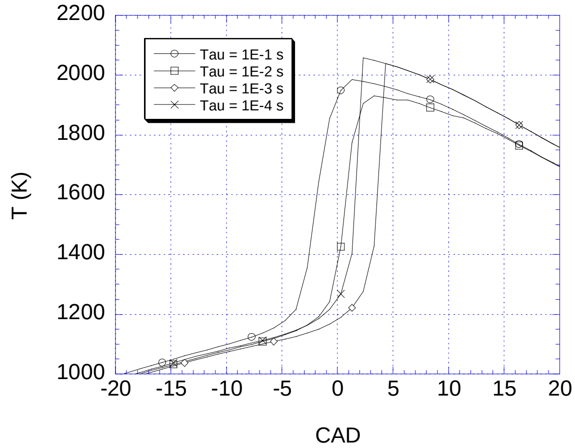

Figure 6: *Sensitivity study on turbulence mixing time scale (τ).*

As one increases the influence of mixing by decreasing τ the ignition is delayed. At a value of τ of 0.001s the mixing is now so efficient that a very large region of the fuel and air

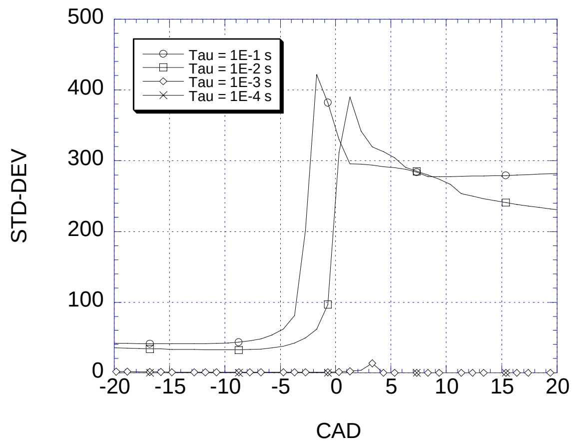

Figure 7: *STD-DEV of temperature histories for the sensitivity study on turbulence time scale.*

mixture will ignite simultaneously. At an even smaller value of τ the situation is in essence similar to the homogeneous case and a very steep slope on the ignition curve is observed.

By observing the STD-DEV of temperature for this study in Figure 7 the mixing effects described above can be better understood. From this graph it is evident that the bulk ignites earlier in the slow mixing cases than the fast mixing cases because it is not cooled by mixing with the boundary layer. As a consequence we find a decrease in the maximum value of the STD-DEV with increasing mixing intensity. As mixing becomes more efficient a time delay between ignition of the colder and hotter spots is noticed.

To observe the effects of mixing in the fast mixing cases Figure 8 is useful. For τ = 0.001s the mixing is close to perfect before ignition and the STD-DEV is an order of magnitude smaller than for the two slow mixing cases. For τ = 0.0001s the mixing is so fast that no STD-DEV reading is noticeable.

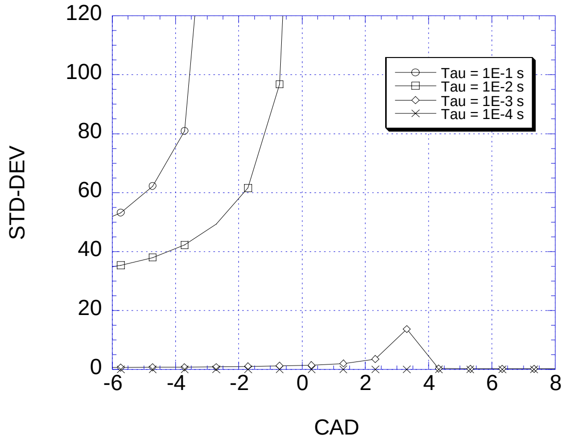

Figure 8: *STD-DEV of temperature. Close-up on the faster mixing cases.*

CONCLUSION

In the present work a new model for the numerical simulation of the combustion process in the HCCI engine has been presented. This model is based on the PaSPFR-IEM model. It is capable of simulating inhomogeneities in the cylinder caused by the thermal boundary layer adjacent to the cylinder walls.

The model results have been verified against engine measurements and results from a PFR model. Generally the new model shows very promising results by significantly improving the results from the PFR model. The simulated ignition curves for temperature and pressure are in very good agreement with the experiments. The modeling of the boundary layer in the cylinder results in a more "smooth" ignition curve as the cold and hot spots in the cylinder ignite at different times. The STD-DEV of temperature gives evidence that not all of the boundary layer is burnt. This might explain the excess of unburnt hydrocarbons from the HCCI engine. The IEM mixing model, as simplest mixing model, needs to be replaced by more realistic models to simulate the mixing process in the engine.

Furthermore a series of sensitivity studies have been carried out where the consequences of different intensities of turbulent mixing have been investigated. The ignition delay time is sensitive to the mixing times. Very slow mixing will result in early ignition of the hot spots followed by a delayed ignition of the colder ones. Very fast mixing will produce a case similar to the homogeneous case.

Future work will include the implementation of a more detailed mixing model e.g. the Curl mixing model. This will increase the demand on CPU-time but will give a more accurate description of the mixing processes taking place in the cylinder. Further experimental results will verify the boundary layer model as used in this work.

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