CONTROL-ORIENTED MODEL OF ISOOCTANE HCCI COMBUSTION

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Abstract: A mathematical engine model is developed in this paper to study the operation process in HCCI engines. Isooctane is used as fuel for testing in this model. Two-step reaction mechanisms are implemented to model combustion process and heat transfer process is also included. Results from this model show good correlation with experiment with respect to combustion phasing, pressure rise and peak pressure. Some control strategies could be potentially developed to stabilize HCCI combustion based on this model. *Copyright © 2005 IFAC*

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1. INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) is an alternative piston-engine combustion process that can provide efficiencies as high as direct-injection diesel engines while, unlike diesel engines, producing ultra-low oxides of nitrogen (*NOx*) and particulate matter emissions. HCCI engines operate on the principle of having a diluted and premixed charge that reacts and burns volumetrically when the cylinder is compressed by the piston. Significant improvement is necessary before an HCCI engine could compete with SI and CI engines in the market. Expanding the controlled operation of an HCCI engine over a wide range of speeds and loads is probably the most difficult hurdle facing HCCI engines. These control issues become particularly challenging during rapid transients.

In recent years, models of variable resolution have been developed as a means to understand the fundamental concepts underlying HCCI combustion in real engine geometries. The simplest approach to model HCCI follows a thermo-kinetic, zero-dimensional formulation in a single homogeneous zone. Najt and Foster (1983) first developed this type of model to help analyze experiment work on a premixed-charge, compression-ignited CFR engine. Recent examples of zero-dimensional models use more sophisticated and detailed chemical kinetics (e.g., Dec, 2002). In most cases, these models do not calculate the dynamic breathing process, but instead rely on idealized charging calculations or estimates made from experiments to define the initial conditions at the start of compression. Fiveland and Assanis (2000) among others have combined the single zone approach with existing zero-dimensional engine models to provide accurate estimates of the effects of the gas exchange process and have used the resulting simulations to evaluate unconventional engine concepts or variable valve timing strategies. Besides single-zone models, other sophisticated and comprehensive HCCI engine models have also been developed in recent years. However, most of these

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models involve either detailed chemical kinetics or high-order equations, which make it difficult to synthesize controllers based on them. Shaver *et al.* (2003) developed a HCCI engine model with simplified combustion mechanisms to investigate control strategies. However, heat transfer effects are assumed to have no implications on the combustion events within their model.

In this paper, an ordinary differential equation based model is proposed for HCCI engine operation. Wall heat transfer process is included in the model. Simulation results indicate that this ODE model yields good match with experimental data published by Christensen and Johansson (1998). Hence, this model is a good candidate to be used for future model based HCCI engine control design.

2. MODEL OF HCCI OPERATION

The model described here is a single-zone model which is based on the first law of thermodynamics and mass balances in an open system. Steady-state compressible flow relations are used to model the valve flow during the induction and exhaust stages of the cycle. Two-step reaction mechanisms with Arrhenius reaction rates are implemented in combustion chemistry modeling. Cylinder wall heat transfer is modeled with Woschni's (1967) heat transfer correction.

2.1 Cylinder Volume Change Rate

The cylinder volume change is solely a function of the cylinder bore and the change of vertical displacement which is governed by the geometry of the crank structure. The cylinder volume change rate is

$$\dot{V} = \frac{\pi B^2}{4}\left(a\sin\theta + \frac{a^2\sin\theta\cos\theta}{\sqrt{l^2 - a^2\sin^2\theta}}\right)\dot{\theta},$$

where V is the cylinder volume, B is the cylinder bore, θ is the crank angle, a is half of the stroke length, l is the connecting rod length. $\dot{\theta}$ is the rotating speed of the crankshaft.

2.2 Mass Flow Rate

The mass flow through the valves consists of flow from intake manifold to cylinder and flow from cylinder to exhaust manifold. Equations for these mass flow rates are developed using compressible, steady state, one-dimensional, isentropic flow analysis for a restriction (Heywood, 1988). For the intake mass flow

$$\dot{m}_1 = \begin{cases} \dfrac{c_D A_1 p_0}{\sqrt{RT_{in}}}\left(\dfrac{p}{p_0}\right)^{1/\gamma_1}\sqrt{\dfrac{2\gamma_1}{\gamma_1 - 1}\left[1 - \left(\dfrac{p}{p_0}\right)^{(\gamma_1-1)/\gamma_1}\right]}, & \left(\dfrac{p}{p_0} > \left(\dfrac{2}{\gamma_1+1}\right)^{\gamma_1/(\gamma_1-1)}\right) \\ \dfrac{c_D A_1 p_0}{\sqrt{RT_{in}}}(\gamma_1)^{1/2}\left(\dfrac{2}{\gamma_1+1}\right)^{(\gamma_1+1)/2(\gamma_1-1)}, & \left(\dfrac{p}{p_0} \le \left(\dfrac{2}{\gamma_1+1}\right)^{\gamma_1/(\gamma_1-1)}\right) \end{cases},$$

and for the exhaust mass flow

$$\dot{m}_2 = \begin{cases} \dfrac{c_D A_2 p}{\sqrt{RT}}\left(\dfrac{p_0}{p}\right)^{1/\gamma_2}\sqrt{\dfrac{2\gamma_2}{\gamma_2 - 1}\left[1 - \left(\dfrac{p_0}{p}\right)^{(\gamma_2-1)/\gamma_2}\right]}, & \left(\dfrac{p_0}{p} > \left(\dfrac{2}{\gamma_2+1}\right)^{\gamma_2/(\gamma_2-1)}\right) \\ \dfrac{c_D A_2 p}{\sqrt{RT}}(\gamma_2)^{1/2}\left(\dfrac{2}{\gamma_2+1}\right)^{(\gamma_2+1)/2(\gamma_2-1)}, & \left(\dfrac{p_0}{p} \le \left(\dfrac{2}{\gamma_2+1}\right)^{\gamma_2/(\gamma_2-1)}\right) \end{cases}.$$

where p_0 is the intake manifold pressure, assumed to be atmospheric, and p is the cylinder pressure. T_{in} is the intake mixture temperature, and T is the cylinder temperature. R is the gas constant. A is the cross-sectional area of the valves. γ is the ratio of specific heats. C_D is the discharge coefficient. For a fully opened poppet valve the discharge coefficient is usually around 0.7 (Stiesch, 2003).

2.3 Chemical Model of Combustion Process

Westbrook and Dryer (1981) derived two-step reaction mechanisms with hydrocarbon fuels. The two-step mechanisms for isooctane/air mixture combustion can be expressed as

$$C_8H_{18} + 8.5(O_2 + 3.773N_2) \rightarrow 8CO + 9H_2O + 32.07N_2$$

$$CO + 0.5O_2 \rightarrow CO_2.$$

The rate of C_8H_{18} and CO reactions are expressed by three-parameter Arrehenius functional form, as

$$\left[\dot{X}_{C_8H_{18}}\right] = -1.13\times10^{10}\exp\left(-30/R_uT\right)*\left[X_{C_8H_{18}}\right]^{0.25}*\left[X_{O_2}\right]^{1.5}$$

$$\left[\dot{X}_{CO}\right] = -1.0\times10^{14.6}*\exp\left(-40/R_uT\right)*\left[X_{CO}\right]^{1}*\left[X_{H_2O}\right]^{0.5}*\left[X_{O_2}\right]^{0.25}$$

$$+5\times10^{8}*\exp\left(-40/R_uT\right)*\left[X_{CO_2}\right]^{1}.$$

The reaction rates of other species concentration can be derived by inspection of the two-step mechanism equations for isooctane/air combustion. As the combustion speed in HCCI engines is very fast and normally happens in several crank degrees, the cylinder volume can be assumed constant during combustion period. Then $\left[\dot{X}_{i,rxn}\right] = \dfrac{\dot{N}_{i,rxn}}{V}$.

2.4 Species Concentration Rate

The concentration of species i in the cylinder can be expressed as $[X_i] = \dfrac{N_i}{V}$, where N_i is moles of species i in the cylinder, V is the cylinder volume. The rate of change of concentration for species i, $\left[\dot{X}_i\right]$ is

$$\left[\dot{X}_i\right] = \frac{\dot{N}_i}{V} - \frac{[X_i]\dot{V}}{V},$$

where $\dfrac{\dot{N}_i}{V}$ is the rate of change of moles of species i per unit volume and $\dfrac{\dot{N}_i}{V} = \dfrac{\dot{N}_{i,rxn}}{V} + \dfrac{\dot{N}_{i,gx}}{V}$, where $\dfrac{\dot{N}_{i,rxn}}{V}$ is the rate of change of moles of species i per unit volume due to the combustion reactions, and $\dfrac{\dot{N}_{i,gx}}{V}$ is due to flow through the inlet and exhaust valves (gas exchange processes). The combustion reaction

rate, $\frac{\dot{N}_{i,rxn}}{V}$, is determined through the use of two-step combustion chemistry mechanism as described before. Given the mass flow rates described previously, $\frac{\dot{N}_{i,gx}}{V}$ can be found using the species mass fractions

$$\frac{\dot{N}_{i,gx}}{V} = \frac{\dot{N}_{i,1}}{V} - \frac{\dot{N}_{i,2}}{V},$$

where $\frac{\dot{N}_{i,1}}{V} = Y_{i,1}\frac{\dot{m}_1}{MW_i \times V}$, $\frac{\dot{N}_{i,2}}{V} = Y_{i,2}\frac{\dot{m}_2}{MW_i \times V}$.

Here $\dot{m}_1$ is the mass flow rate from intake manifold to cylinder, $\dot{m}_2$ is the mass flow rate from cylinder to exhaust manifold, $Y_{i,1}$ and $Y_{i,2}$ are the mass fractions of species i in the inlet manifold and exhaust manifold, respectively, MW_i is the molar weight of species i. It is assumed that a homogeneous mixture is present in the intake manifold with air/fuel equivalence ratio known. Further, if using two-step reaction mechanisms, there are five species in combustion products: CO_2, CO, H_2O, N_2 and O_2. It is assumed no fuel of C_8H_{18} left after combustion.

2.5 Wall Heat Transfer Rate

Wall heat transfer effect is considered in this model, unlike previous works by other researchers (Shaver *et al.*, 2003). The heat transfer rate between the gas in the cylinder and the cylinder wall can be described by

$$\dot{Q} = hA_w(T_w - T),$$

where h is the heat transfer coefficient, A_w is the wall surface area, T_w is the mean wall temperature, T is the cylinder gas temperature. The heat transfer coefficient is described by Woschni (1967).

$$h = CB^{m-1}p^m v^m T^{0.75-1.62m},$$

where C is a constant, B is the cylinder bore, v is the average cylinder gas velocity. The average cylinder gas velocity v is determined by Woschni as

$$v = \left[C_1\bar{S}_p + C_2\frac{V_d T_r}{p_r V_r}(p - p_m)\right],$$

where V_d is the displaced volume, $\bar{S}_p$ is the mean piston speed ($=2LN$, L is the stroke and N is the engine rotation speed), p is the instantaneous cylinder pressure, p_r, V_r, T_r are the working-fluid pressure, volume, and temperature at some reference state (say inlet valve closing or start of combustion), p_m is the motored cylinder pressure at the same crank angle as p, C_1 and C_2 are constants.

2.6 Conservations of Mass and Energy

The first law of thermodynamics for an open system and the ideal gas law are combined to describe mass and energy balances in the engine cylinder. The change of mass contained within the cylinder is equal to the difference between all entering and exiting mass flows, $\dot{m}_1$ and $\dot{m}_2$ respectively:

$$\frac{dm}{dt} = \sum \dot{m}_{1,i} - \sum \dot{m}_{2,i}.$$

The energy balance for the cylinder becomes

$$\frac{dE}{dt} = \dot{Q} - \dot{W} + \sum \dot{m}_{1,i}h_i - \sum \dot{m}_{2,i}h_i,$$

where $\dot{Q}$ is the rate of heat transferred to the cylinder from combustion, $\dot{W}$ is the rate of mechanical work done by the piston, h_i is the enthalpy of species in the intake and exhaust manifold. The work rate done by the piston, $\dot{W}$, can be expressed as $\dot{W} = mp\dot{v}$, where v is the specific volume of the gases in the cylinder. A differential equation for the temperature of the gas inside the cylinder can be derived according to conservations of mass and energy.

3. RESULTS AND DISCUSSION

3.1 Experimental Work by Other Researchers

Christensen and Johansson (1998) investigated the effect of mixture quality on HCCI combustion. One of the fuels they used in their experiments is isooctane, with three different fuel flow rates. They measured the cylinder pressure for all operating conditions with and without EGR. The cylinder pressure was recorded for 100 cycles, every 0.2 degrees of crank angle with a pressure transducer mounted on the cylinder head. The HCCI engine used in experiments was converted from a Volvo TD100 series diesel engine. The key engine parameters are summarized in Table 1.

Table 1: Geometric properties of engine

Displaced Volume(cm^3)	**1600**
Bore(mm)	**120.65**
Stroke(mm)	**140**
Connecting Rod(mm)	**260**
Inlet Valve Diameter(mm)	**50**
Exhaust Valve Diameter(mm)	**46**
Exhaust Valve Open	**39° BBDC**
Exhaust Valve Close	**10° BTDC**
Inlet Valve Open	**5° ATDC**
Inlet Valve Close	**13° ABDC**

Table 2: Conditions of engine operation

Case	**A**	**B**	**C**
Fuel Flow Rate(mg/cycle)	**24.8**	**29.6**	**34.9**
Inlet Temperature(K)	**388**	**388**	**388**
Boost Pressure(bar)	**0**	**0**	**0**
Compression Ratio	**18**	**18**	**18**
Air/Fuel Ratio λ	**3.5**	**2.9**	**2.5**

Table 2 summarizes conditions of engine operation at three different fuel flow rates. The HCCI engine model described in this paper adopted all engine parameters and operation conditions from Tables 1

and 2 to make it possible to compare the model simulation results with the experimental results published by Christensen and Johansson (1998).

3.2 Comparison of Measured and Predicted Cylinder Pressure

In Figures 1, 2 and 3, predicted cylinder pressure profiles are compared with measured pressure at three fuel flow rates, which are listed in Table 2. All of the three cases are operated at an intake mixture temperature of 388 K without boosted pressure. The air/fuel ratio decreases with higher fuel flow rate (See Table 2). Compression ratio is kept at 18.

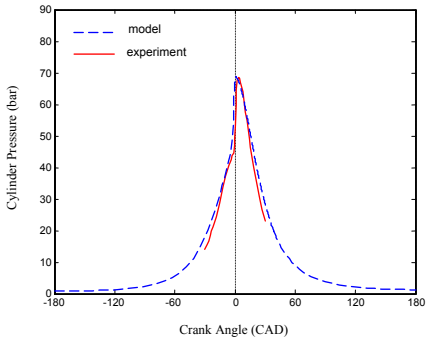

Figure 1: Comparison of predicted cylinder pressure with measured data as function of CAD (fuel flow rate: 24.8 mg/cycle).

By using this model, the essential characteristics of HCCI combustion are captured and the ignition and combustion phasing are also predicted reasonably well. The simulations track the compression and combustion well for all three cases. The predicted peak pressures are nearly equal to the experimental

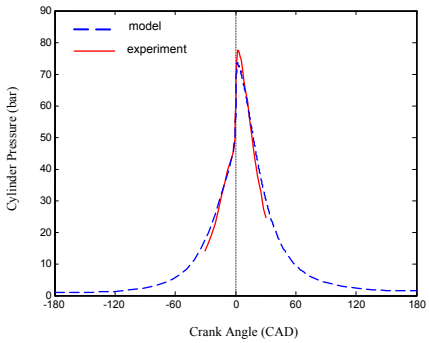

Figure 2: Comparison of predicted cylinder pressure with measured data as function of CAD (fuel flow rate: 29.6 mg/cycle).

data and the predicted ignition timing is within 4º of the measured value. Simulations exhibit a little problem at adequately matching the trapped in-cylinder mass in compression stroke. Also, there are some differences between the calculated pressure curves and those representing experimental data during the expansion strokes. The main reason is that this HCCI model described here is a single-zone model. Although the single-zone model has proven very successful in predicting start of combustion and providing reasonable estimates for peak cylinder

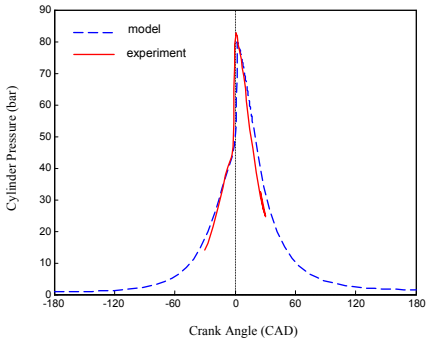

Figure 3: Comparison of predicted cylinder pressure with measured data as function of CAD (fuel flow rate: 34.9 mg/cycle).

pressure, indicated efficiency and NOx emissions (Aceves *et al*., 2001), for very accurate predictions of the engine operation (including expansion process), the multi-zone model should be used at the cost of longer running time.

3.3 Predicted Results with and without Heat Transfer

The Woschni's heat transfer coefficient is implemented in the HCCI engine model. The effects of heat transfer model on predicted pressure and temperature are discussed in this section.

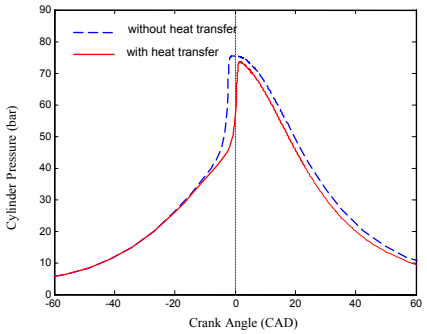

Figure 4: Comparison of predicted cylinder pressure with and without wall heat transfer as function of CAD (fuel flow rate: 29.6 mg/cycle).

The predicted in-cylinder gas pressure and temperature with and without heat transfer for the fuel flow rate of 29.6 mg/cycle are shown in Figures 4 and 5. Without heat transfer model, the ignition timing is advanced 3-5º CAD with higher peak pressure and peak temperature. The predicted cylinder pressure and temperature without heat transfer during expansion stroke are higher than with heat transfer. In Figure 4, it can be seen that the pressure without heat transfer is about 2-3 bar higher than with heat transfer at 60º ATDC. Similarly in Figure 5, the predicted cylinder temperature without heat transfer is more than 150 K than that with heat transfer at 60º ATDC, which leads to higher predicted exhaust temperature.

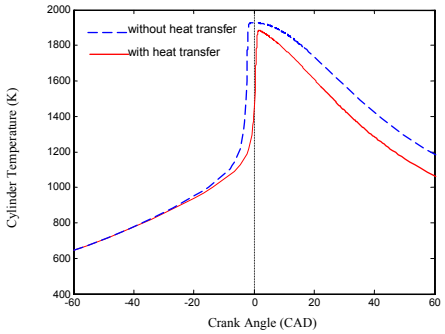

Figure 5: Comparison of predicted cylinder temperature with and without wall heat transfer as function of CAD (fuel flow rate: 29.6 mg/cycle).

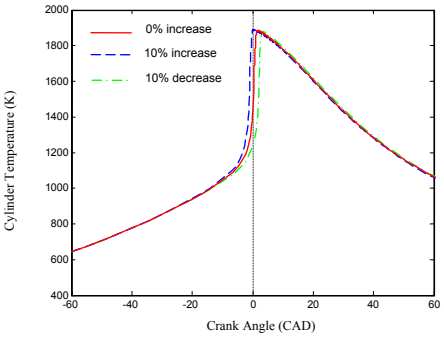

Figure 6: Comparison of predicted cylinder temperature with different pre-exponential factor as function of CAD (fuel flow rate: 29.6 mg/cycle).

Table 3: Comparison of experimental and predicted exhaust temperature with and without heat transfer

Case	A	B	C
Fuel Flow Rate(mg/cycle)	**24.8**	**29.6**	**34.9**
$T_{\exp}$ **(K)**	**503**	**528**	**538**
T_{mod} **with H.T. (K)**	**600**	**643**	**681**
T_{mod} **without H.T. (K)**	**689**	**741**	**788**

Table 3 compares the predicted and experimental exhaust temperature for the three fuel flow rates. In this HCCI model, the cylinder temperate at the end of expansion stroke (BDC) is taken as the predicted exhaust temperature, as the exhaust valve of the experimental engine opens from 39º BBDC to 10º BTDC (See Table 1). It can be found that with heat transfer the predicted exhaust temperature is about 100 K higher than experimental one. Without heat transfer, the predicted exhaust temperature is higher than experimental data about 200 K. The difference increases as fuel flow rate increases. Although the single-zone model has proven very successful in predicting start of combustion and providing reasonable estimates for peak cylinder pressure, it seems that the single-zone model has some problems at predicting engine operation in expansion stroke. The calculated peak temperatures with heat transfer are 1750, 1880 and 2000 K for three fuel flow rates respectively. Such peak temperatures are significantly lower than those in typical gasoline or diesel engines and are the main reason for the low NOx emissions for the HCCI engine.

3.4 Sensitivity Analysis

The pre-exponential factor A in Arrehnius form should be calibrated for some reference condition with comparisons between computed and experimental data. Also the constant C in Woschni's heat transfer coefficient is adopted from a recent research result. The sensitivities of model outputs on these two parameters are presented in this section.

According to Westbrook and Dryer (1981), the pre-exponential factor A in simulation should be calibrated for comparison with experimental data. After comparing with the experimental data, the pre-exponential factor A in isooctane oxidation equation is taken as $1.13\times10^{10}\left(gmol/cm^3-s\right)$. For studying the effect of the pre-exponential factor on model output, comparison of predicted cylinder temperatures with different pre-exponential factors are illustrated in Figures 6. Increasing 10% of A and decreasing 10% of A are tested in the model. The fuel flow rate of 29.6 mg/cycle is used in tests.

It is seen in Figure 6 that when increasing 10% of A, the ignition timing is advanced about 2-3º CAD. The peak temperature shows a little higher value with increase of pre-exponential factor. Decreasing 10% of A shows reverse effects: the ignition timing is retarded. There is no significant difference in exhaust temperature while either increasing or decreasing the pre-exponential factor.

The constant C in the heat transfer coefficient equation is also adjusted in simulation to represent the experimental results better. Here in the HCCI model, the constant C is taken as 127.93 according to Stiesch (2003). The effect of this constant on the predicted cylinder temperature is shown in Figure 7. Either increasing or decreasing 10% of C has no obvious effects on combustion temperature. Combustion timings in any of the two cases differ in less than 2º CAD. It is concluded that the model output is less sensitive to this constant.

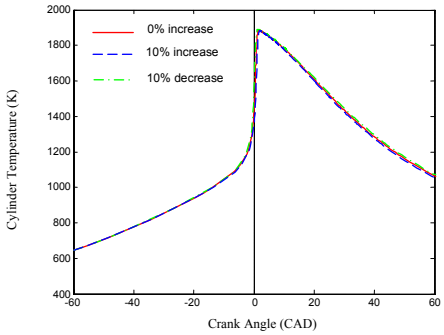

Figure 7: Comparison of predicted cylinder temperature with different heat transfer coefficient as function of CAD (fuel flow rate: 29.6 mg/cycle).

4. CONCLUSIONS

A mathematic HCCI engine model is developed in this paper to study HCCI engines operation and control strategy. Dynamic breathing process is calculated in this model instead of relying on idealized charging calculations to define the initial conditions at the start of compression. Two-step reaction mechanisms are implemented in combustion chemistry modeling where Arrhenius reaction rates are used. Woschni's correction is used to model cylinder wall heat transfer. Three different fuel flow rates are tested in this model. Simulated results from the HCCI engine model are compared with published experimental data from one modified heavy-duty diesel engine. By using this model, the essential characteristics of HCCI combustion are captured and the ignition and combustion phasing are also predicted reasonably well. The simulation also shows that with Woschni's heat transfer model, the HCCI engine model predicts engine operation better, especially at compression stroke. Without heat transfer model, the predicted exhaust temperature is about 200 K higher than experimental data. The HCCI engine model illustrated in this paper could be used to carry out parameter studies and contributes to the development of the combustion control strategies, such as VCR and VVT controllers. In future work, advanced valve actuation strategies could be investigated to incorporate HCCI into a multi-combustion-mode engine capable of meeting consumer demands for power, efficiency and emissions.

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