

## **EFFECT OF DIFFERENT HEAT TRANSFER MODELS ON A DIESEL HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINE**

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### **ABSTRACT**

Homogeneous charge compression ignition (HCCI) engine technology is relatively new and has not matured sufficiently to be commercialized compared with conventional engines. It can use spark and compression ignition engine configurations, capitalizing on the advantages of both: high engine efficiency with low emissions levels. However, the combustion behavior in an HCCI engine is difficult to predict because it has no spark plug or injector. The chemical kinetics mechanism influences the combustion with some heat losses to the cylinder wall. The effect of different heat loss models in a diesel HCCI engine has to be investigated further. A single-zone thermodynamics model was used in this study along with three different heat loss models: Woschni, modified Woschni, and Hohenberg correlations. It was found that the difference in heat loss models leads to a big difference in the heat flux, and the modified Woschni model has the highest heat flux among these models. The effects of the different scaling factor and characteristic velocity were also investigated. The study concluded that the modified Woschni model produced more accurate results, while the Woschni and Hohenberg models require more tuning of constants before they can be used in a diesel HCCI engine.

**Keywords:** Diesel; HCCI; single-zone; thermodynamics model; heat transfer.

### **INTRODUCTION**

Homogeneous charge compression ignition (HCCI) engines have been an active research area recently (Zhong et al., 2005; Naiki, Iida, & Lhomme, 2010; Yu et al., 2007; Janhunen, 2012; Yun, Wermuth, & Najt, 2011) due to their advantages in reducing emissions levels. Regulatory bodies, such as those in Europe, the United States and Japan, are imposing stringent vehicle emissions quality standards (Wesselink, Buijsman, & Annema, 2006; EPA, 2000; Popp, 2004). Thus, most automotive manufacturers need to develop hybrid or electric vehicles that can reduce emissions levels. Hybrid vehicles are receiving increasing attention from most manufacturers because they offer advantages including reduced emissions and providing good mileage per fuel tank (Chan, 2002). The HCCI engine has the potential to replace the current conventional engine used in hybrid vehicles. HCCI engines can be considered new technology even though the first research associated with it dates back to Onishi et al. (1979). The combustion is fully controlled by the chemical kinetics instead of by the spark or injection timing as in the spark ignition (SI) or compression ignition (CI) engines respectively. It takes place when the homogeneous mixture has reached the

chemical activation energy and the mixture auto-ignites in multiple spots (Bhaskar, Nagarajan, & Sampath, 2010). The advantages of HCCI engines are: 1) high-efficiency engines due to a high compression ratio (CR), 2) similar or even better power band compared with SI or CI engines, and 3) the ability to operate in any configuration and with any fuels: stationary engines, automobile engines, or small- and large-sized engines. On the other hand, the disadvantages are: 1) difficult to control the ignition timing and achieving cold start (Kong & Reitz, 2003; Ishak, Tahseen, & Rahman, 2013; Soylu, 2005), 2) high levels of unburned hydrocarbons (UHC) and carbon monoxide (CO) (Kong et al., 2003; Nathan, Mallikarjuna, & Ramesh, 2010), and 3) knocking issues if the mixture is relatively inaccurate (Jun et al., 2003; Kong & Reitz, 2003; Nathan et al., 2010).

The use of numerical studies in HCCI engines is becoming a necessity because it can reduce costs related to experimental work. Computational fluid dynamics (CFD) approaches are used to obtain more accurate results at the expense of computational costs, while thermodynamics approaches are suitable for fast results that are comparable to experimental results (Babajimopoulos, Lavoie, & Assanis, 2003; Canova et al., 2005). This paper uses the thermodynamics approach to investigate the effect of different heat transfer models on an HCCI engine. The use of an accurate heat transfer model is an essential element for acquiring accurate yet fast results for thermodynamics simulations. Soyhan et al. (2009) studied the effect of similar heat transfer models on a gasoline HCCI engine. However, their HCCI engine model was based on a predicted auto-ignition time, and the auto-ignition time was modeled with no chemical kinetics mechanism employed. Kong and Reitz (2002) reported that the HCCI engine is fully controlled by chemical kinetics. Thus, the use of a chemical kinetics mechanism, which is employed in this study, is important in an HCCI engine model. The auto-ignition time is no longer modeled and is solely dependent on the chemical reaction mechanism to achieve combustion. Another advantage of employing a chemical kinetics mechanism in an HCCI engine model is that any fuel can be represented in the model and is not just limited to gasoline or any specific fuel. This paper consists of four sections, and the thermodynamics model is explained in the next section. Then, the following section discusses the findings of the simulation, and the paper closes with the conclusions in the last section.

## **THERMODYNAMICS MODEL**

A zero-dimensional single-zone model was used to simulate the combustion behavior of a diesel HCCI engine. The zero-dimensional model was initially developed by Assanis and Heywood (1986), but some changes have been made: chemical reaction mechanisms have been added, and a different heat release rate model was used. The thermodynamics properties were assumed to be uniform throughout the combustion chamber. The simulation began from the inlet valve open (IVO) up to the exhaust valve open (EVO). It was coded using MATLAB software combined with a chemical kinetics package.

### **Engine Geometry**

The instantaneous volume at any crank angle position  $\theta$  can be obtained from

$$V = V_c \left[ 1 + \frac{R_c - 1}{2} \left( R + 1 - \cos\theta - \sqrt{R^2 - \sin^2\theta} \right) \right] \quad (1)$$

where  $V_c$  is the clearance volume,  $R_c$  is the compression ratio, and  $R$  is the connecting rod length. Differentiating Eq. (1) with respect to the crank angle, the rate of change of volume is

$$\frac{dV}{d\theta} = V_c \left[ \frac{R_c - 1}{2} (\sin\theta) \left( \frac{1 + \cos\theta}{\sqrt{R^2 - \sin^2\theta}} \right) \right] \quad (2)$$

The change in volume is an important parameter; this equation will be used to determine the piston work.

### Conservation Equations

Three conservation equations are used in this study: mass, energy, and chemical species. Because the thermodynamics system is an open system, the mass flows in and out of the system, affecting the total mass of the chamber

$$\frac{dm}{dt} = \sum_j \dot{m}_j \quad (3)$$

where  $j$  represents each flow in or out of the system. Then the energy equation, which was derived from the first law of thermodynamics equation, is used. After manipulations, the change in temperature is given by

$$\begin{aligned} \frac{dT}{dt} = \frac{1}{\left(\bar{C}_p - \frac{Pv}{T}\right)} & \left[ \left( \frac{Pv \sum_i R_i}{R_u} - \sum_i h_i \right) \frac{dY_i}{dt} - \frac{\dot{m}_{in}}{m} (h - Pv) \right. \\ & \left. + \frac{1}{m} \left( \frac{dQ_h}{dt} - P \frac{dV}{dt} + \sum_j \dot{m}_j h_j \right) \right] \end{aligned} \quad (4)$$

In Eq. (4),  $\bar{C}_p$  is the specific heat at constant pressure,  $P$  is the in-cylinder pressure,  $T$  is the instantaneous in-cylinder temperature,  $v$  is the specific volume,  $R_u$  is the universal gas constant,  $Y_i$  is the mass fraction of species  $i$ ,  $\dot{m}_{in}$  is the mass flow rate into the cylinder,  $h$  is the enthalpy,  $Q_h$  is the heat loss to the cylinder wall, and  $V$  is the instantaneous cylinder volume. Then, the in-cylinder pressure is obtained using the ideal gas equation

$$P = \frac{\rho R_u T}{\overline{W}_{mw}} \quad \text{with} \quad \overline{W}_{mw} = \frac{1}{\sum_{i=1}^n Y_i / W_i} \quad (5)$$

where  $\overline{W}_{mw}$  is the mean molecular weight of the mixture,  $W_i$  is the molecular weight of the  $i$ th species and  $n$  is the total number of species.

The chemical reactions are the source term in the energy equation, where they affect the temperature based on the energy being transferred from one form to another.

Because chemical kinetics fully control HCCI engines, it is critical to model the combustion with a chemical reaction mechanism, rather than a pre-defined ignition point. In this study, a reduced n-heptane mechanism (Seiser et al., 2000) was used to simulate diesel combustion. This was chosen because n-heptane's chemical properties are similar to those of conventional diesel in terms of the cetane number. The mechanism consists of 160 species and 770 elementary reactions. Thus, the change of mass fraction of each species due to chemical reactions is given by

$$\frac{dY_i}{dt} = \dot{\omega}_i W_i \nu, \quad i = 1, \dots, n \quad (6)$$

where  $\dot{\omega}_i$  is the molar production rate of the  $i$ th species.

### Gas Exchange Process

The gas exchange process when the gas exits the inlet valve into the combustion chamber must be accounted for because the simulation begins from the IVO. This process is used to determine the mass flow rate of the mixture to the combustion chamber. A steady-state, one-dimensional isentropic flow is used to model the gas exchange process (Heywood, 1988).

### Heat Transfer Model

Heat is transferred between the cylinder walls and in-cylinder gases through convection and radiation, and for HCCI engines, the radiation effect is neglected (Soyhan et al., 2009). The convective heat transfer rate can be described by Newton's law of cooling (Stiesch, 2003):

$$\frac{dQ_h}{dt} = h_c A_w (T - T_w) \quad (7)$$

where  $h_c$  is the heat transfer coefficient,  $A_w$  is the cylinder wall area and  $T_w$  is the wall temperature. The wall area is the sum of the cylinder wall, piston crown, and cylinder head areas. The heat transfer coefficient has to be modeled, with the model attempting to reproduce the heat release rate obtained from experiments. The effects of different heat transfer coefficient models are studied in this paper, where the models used are the Woschni correlation (Bengtsson, Gafvert, & Strandh, 2004; Woschni, 1967), modified Woschni correlation for HCCI engines (Chang et al., 2004), and Hohenberg correlation (Hohenberg, 1979; Sanli et al., 2008; Zeng & Assanis, 1989).

The Woschni heat transfer coefficient uses bore,  $B$ , as the characteristic length and mean piston speed,  $\overline{S}_p$ , as the characteristic velocity:

$$h_c = 3.26 B^{-0.2} P^{0.8} T^{-0.55} (2.28 \overline{S}_p)^{0.8} \quad (8)$$

In Eq. (8),  $P$  is the instantaneous in-cylinder pressure in bars.

A modified Woschni correlation has been developed for HCCI engines with the measurements taken in the piston crown and cylinder head areas (Chang et al., 2004). The equation then becomes

$$h_c = \alpha_{scaling} L^{-0.2} P^{0.8} T^{-0.73} (v_{tuned})^{0.8} \quad (9)$$

where the characteristic velocity  $v_{tuned}$  is

$$v_{tuned} = C_1 \bar{S}_p + \frac{C_2 V_d T_r}{6 P_r V_r} (P - P_{mot}) \quad (10)$$

The modified Woschni equation uses the instantaneous chamber height,  $L$ , as the characteristic length scale; the temperature exponent is changed to 0.73, and  $\alpha_{scaling}$  is the scaling factor to fit the experimental data. In Eq. (10),  $C_1 = 2.28$  and  $C_2 = 0.00324$  are constants,  $V_d$  is the displacement volume, subscript  $r$  is the reference condition, and  $P_{mot}$  is the motoring pressure: the cylinder pressure without combustion.

The Hohenberg correlation, on the other hand, includes some modifications to the Woschni equation, as it uses instantaneous cylinder volume instead of bore. Apart from that, the characteristic velocity is replaced with the effective gas velocity, and the temperature exponent has also changed. The Hohenberg heat transfer equation is given by (Sanli et al., 2008).

$$h_c = 3.26 P^{0.8} T^{-0.4} V^{-0.06} (\bar{S}_p + 1.4)^{0.8} \quad (11)$$

The difference in heat transfer correlations leads to varying predictions regarding heat loss. Therefore, the combustion behavior is also changed with different heat coefficients. The changes become significant in HCCI engines, where chemical kinetics plays a major role in combustion.

## RESULTS AND ANALYSIS

Validation of the thermodynamics model is required before proceeding with further analysis. The model was validated against experimental data from Guo et al. (2010), with the experiment using HCCI engines fueled with n-heptane. The port-injection approach was used, with the n-heptane injected at the inlet port. Guo et al. (2010) also used a zero-dimensional model to simulate their experiment. Thus, the validation will be compared against their experiment and model. The engine parameters used in this study are shown in Table 1. Because the fuel is port-injected, the mixing effect must be taken into consideration, with the effective intake mixture temperature set 20°C higher than the desired intake temperature (Guo et al., 2010). Therefore, the intake temperature in this study was increased to 333K for the intake temperature of 313K. The validation result is shown in Figure 1, where it is compared with the experiment and another single-zone model from Guo et al. (2010). The validated result was completed using a modified Woschni heat transfer coefficient with an air-to-fuel ratio (AFR) of 50. The predicted maximum in-cylinder pressure is evidently slightly higher than that of the experiment due to the limitation of the thermodynamics model: the entire combustion chamber is assumed to be homogeneous. Overall, the predicted in-cylinder pressure is in good agreement with the experimental data.

The in-cylinder pressure is predicted differently when using different heat transfer coefficient models, as shown in Figure 2(A). Both the Woschni and Hohenberg models over-predicted the combustion phasing by having an advanced ignition about

5°CA earlier than the experiment did. The modified Woschni equation, on the other hand, agreed well with the experiment despite having a slightly higher maximum in-cylinder pressure compared with the experiment. In a diesel HCCI engine with a reduced compression ratio, a cool flame phenomenon, which is called the low temperature reaction (LTR), occurred at a temperature below the auto-ignition temperature and created a two-stage ignition, with the LTR and HTR (high temperature reaction) (Kim & Lee, 2007; Neely, Sasaki, & Leet, 2004). The LTR region was found to be advanced for all heat transfer coefficient models at about 340°CA. The LTR region was found to be about 800 K, which is the same as reported by Kim and Lee (2007). The HTR region, on the other hand, begins at about 900 K, as shown in Figure 2(B). This is in agreement with other studies, where the HTR region began at about 900–1050 K (Epping et al., 2002; Zheng et al., 2001).

Table 1. Engine parameters used in the current study; ATDC is after top dead center, ABDC is after bottom dead center, BBDC is before bottom dead center (Guo et al., 2010).

Engine Parameters	Value and unit
Cylinder bore	82.55 mm
Stroke	114.3 mm
Connecting rod length	254 mm
Compression ratio (CR)	10
Engine speed	900 rpm
Inlet valve open (IVO)	10° CA ATDC
Inlet valve closed (IVC)	36° CA ABDC
Exhaust valve open (EVO)	40° CA BBDC
Exhaust valve closed	5° CA ATDC

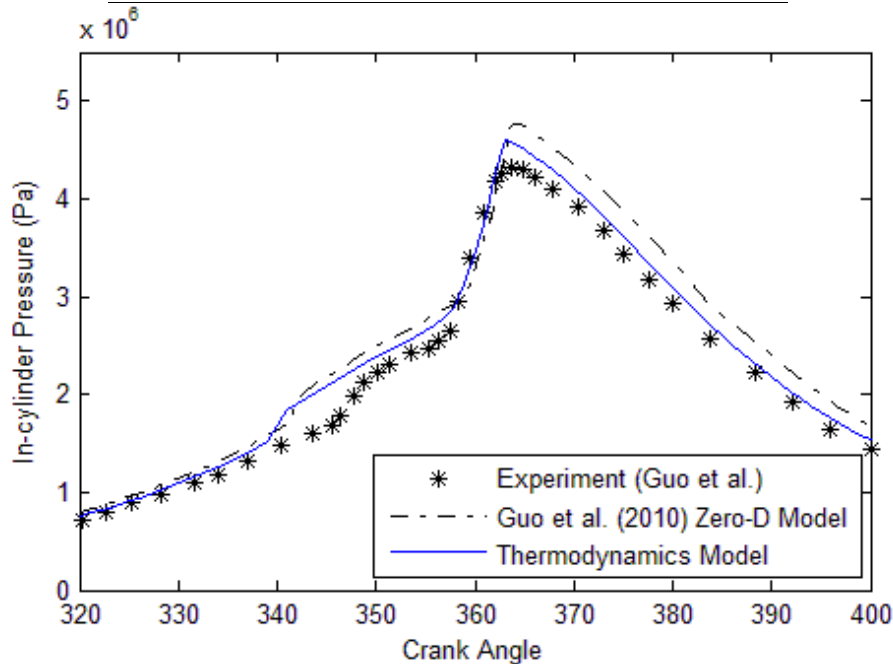


Figure 1. Comparison between single-zone thermodynamics model (with modified Woschni heat transfer model) with experimental data and another single-zone model (Guo et al., 2010). CR=10.0, N=900 rpm,  $T_{in}=40^{\circ}\text{C}$ ,  $P_{in}=95\text{ kPa}$ , AFR=50.

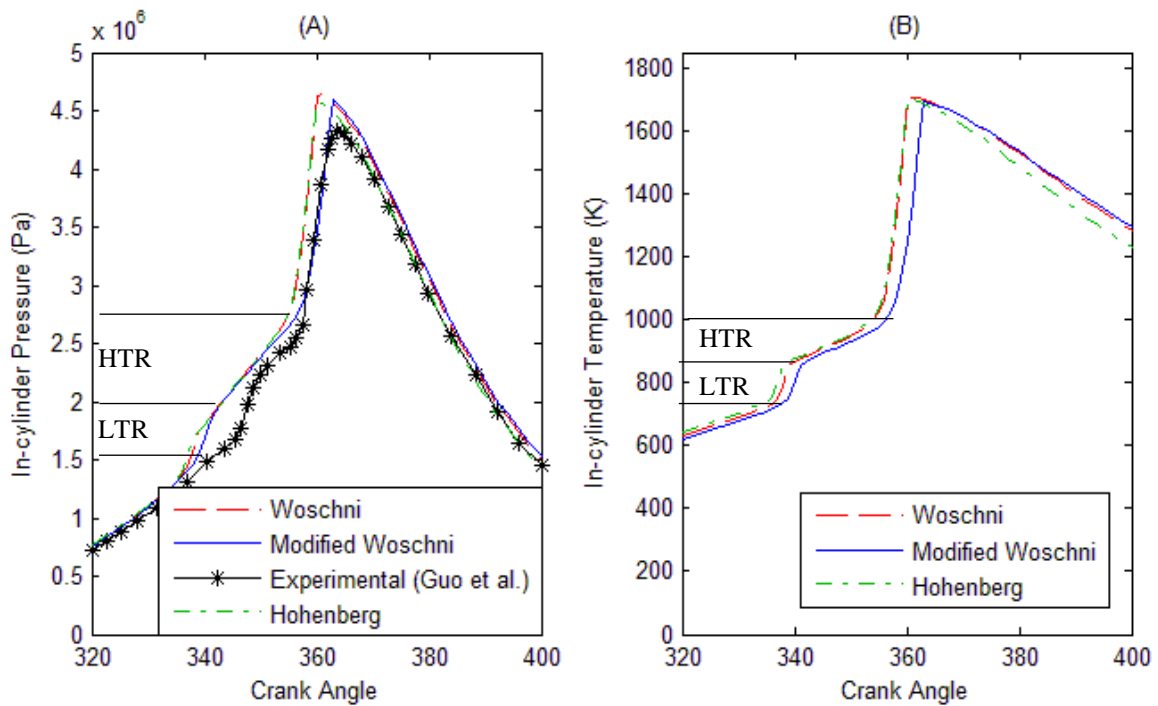


Figure 2. Combustion phasing for different heat transfer coefficient models showing high temperature region (HTR) and low temperature region (LTR). In-cylinder pressure on the left and temperature on the right for different heat transfer coefficient models.

## Heat Fluxes

The history of the heat transfer coefficient and the heat release rate among all models are shown in Figure 3, with the maximum values varying from 9 to 278  $\text{W}/\text{m}^2\text{K}$ . The difference in this value is due to a difference in the scaling factor, velocity characteristic, and temperature exponent. The modified Woschni equation has the highest heat transfer coefficient value (with the highest scaling factor, which is 194.7), which causes it to have the highest heat release rate, as in Figure 3. The heat transfer coefficient traces were changed when the same scaling factor was used for all models, as shown in

Figure 4. The Hohenberg correlation has the highest heat transfer coefficient, compared with the other two models, as a result of the difference in the temperature exponent used in the model. The heat flux decreases when the piston is in a downward motion, and during the intake process, the heat flux is minimal. This shows that heat is being added to the chamber during the intake process, when the wall temperature is slightly higher than the in-cylinder temperature. However, the heat flux increases when the piston is in the compression process. A high heat transfer coefficient causes too much heat loss to the cylinder wall, and this shows that the Hohenberg model causes too much energy to be wasted when the piston is at TDC. Therefore, a high scaling factor is not suitable for the Hohenberg model.

Improper characteristic velocity causes incorrect heat loss to the cylinder wall. The piston is in a downward and upward motion, so the piston's instantaneous velocity

is not the same across the crank angle ranges. The instantaneous piston speed is at minimum when the piston is at TDC and BDC, and it is at maximum when the piston is in the middle of the stroke. Therefore, in this case, the characteristic velocity could be different across the stroke range. However, the Woschni and Hohenberg models assumed that the characteristic velocity is constant for all of the crank angle ranges, as shown in Figure 5. The modified Woschni equation, on the other hand, uses a different approach, where the characteristic velocity varies across the engine cycle.

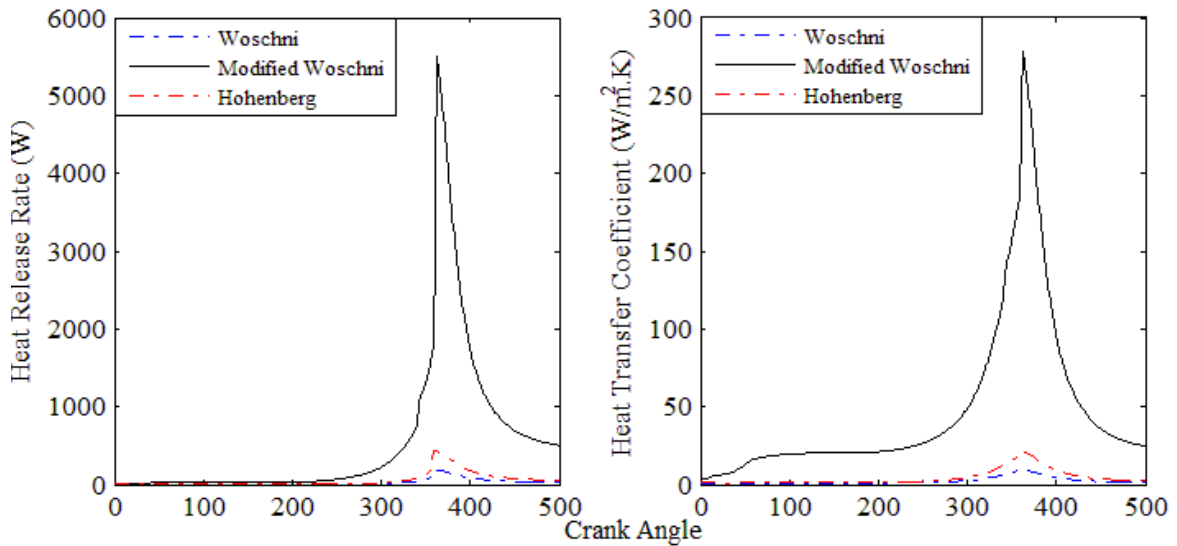


Figure 3. Heat release rate (left) and heat transfer coefficient (right) comparison among Woschni, modified Woschni and Hohenberg models.

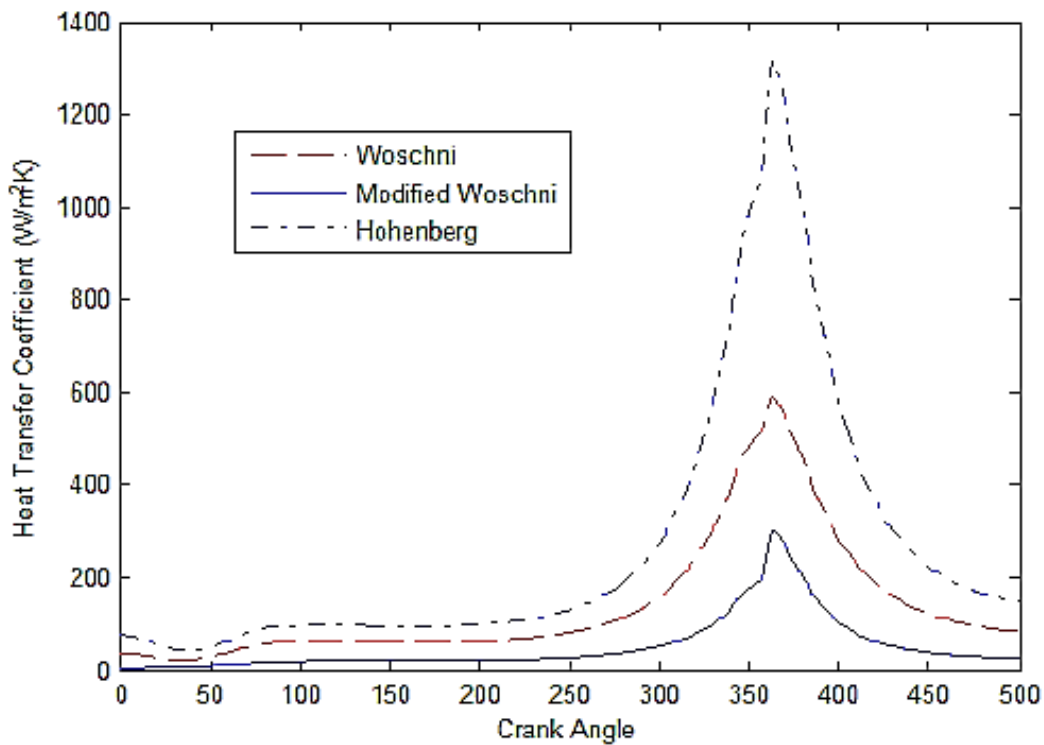


Figure 4. Comparison of heat transfer coefficients with same scaling factor.



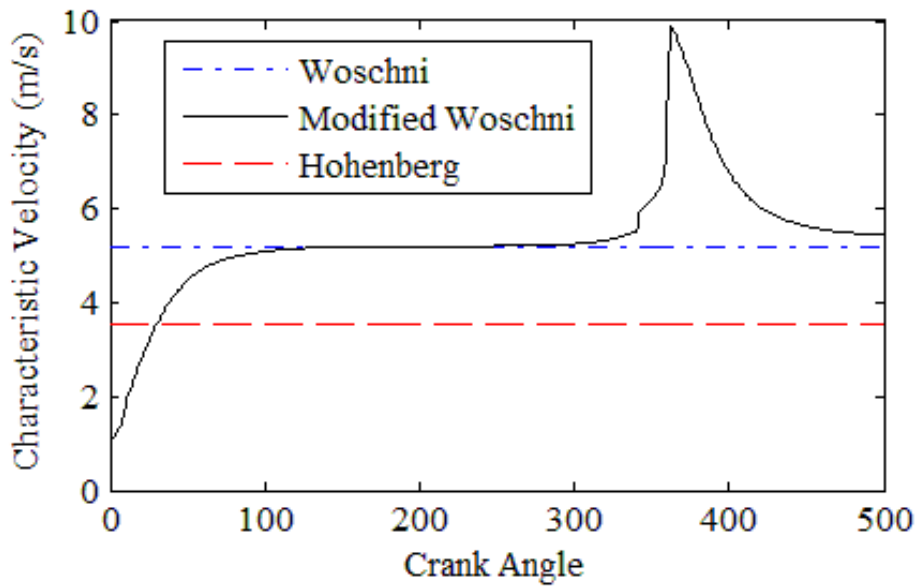


Figure 5. Comparison of characteristic velocity between the Woschni, modified Woschni, and Hohenberg models.

### Heat Transfer Behavior of Different AFR

A diesel HCCI engine operates in a lean condition, where the actual AFR is greater than the stoichiometric AFR of 14.5. In a high-load operation, the AFR is reduced toward the rich zone, while the AFR is higher when the engine is in a low load. Heat loss effects for all models were tested with varying AFRs. Both the Woschni and Hohenberg models yielded higher peak in-cylinder pressure compared with the modified Woschni equation for both different AFRs, as shown in

Figure 6.

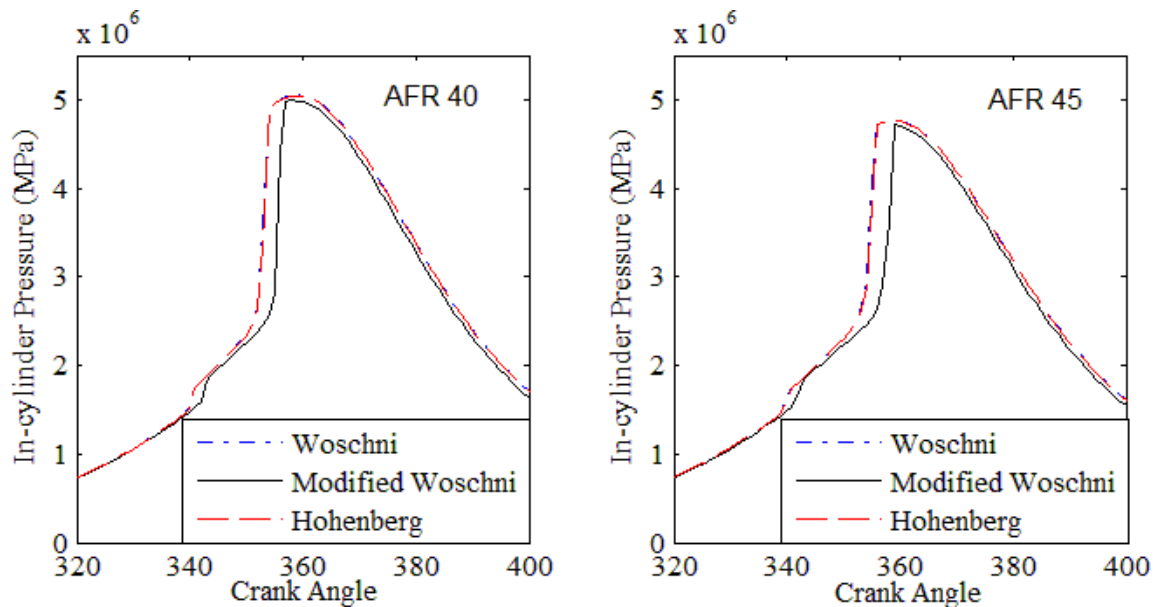


Figure 6. In-cylinder pressure comparison with different AFRs and different heat transfer coefficient models, CR=10.0, N=900 rpm,  $T_{in}=40^{\circ}C$ ,  $P_{in}=95$  kPa.

The LTR region is advanced for both the Woschni and Hohenberg models and subsequently for the main combustion (HTR) region. A low heat transfer coefficient for the Woschni and Hohenberg models, as shown in Figure 7, leads to more energy being trapped in the combustion chamber. Therefore, the combustion is advanced because the chemical kinetics acquires more energy to react. A constant gas velocity term for the Woschni and Hohenberg models causes improper heat loss prediction and requires more tuning to achieve a desirable result. The modified Woschni equation agreed well with the experiment and can be used for further analysis of diesel HCCI engines.

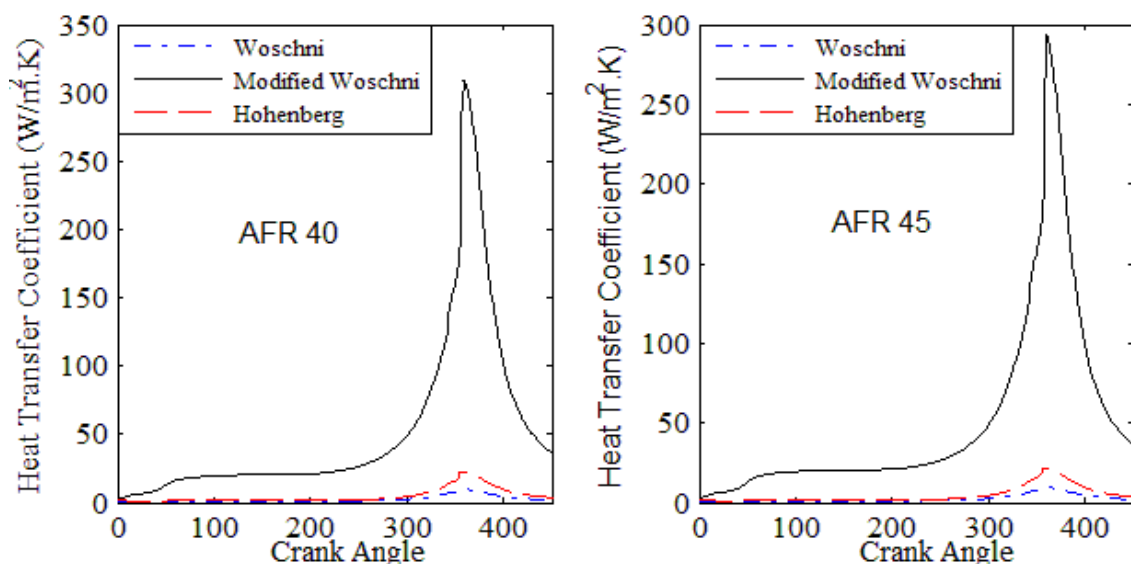


Figure 7. Heat release rate comparison with varying AFRs and different heat transfer coefficient models, CR=10.0, N=900 rpm,  $T_{in}=40^{\circ}C$ ,  $P_{in}=95$  kPa.

### CONCLUSIONS

A study of the heat flux analysis of a diesel HCCI engine is the objective of this paper. A single-zone thermodynamics model is used and validated against the experiment. The thermodynamics model is in agreement with the experiment. Three different heat transfer coefficient models were investigated: the Woschni, modified Woschni, and Hohenberg models. The models used different characteristic length and velocity scales as well as different temperature exponents. These differences lead to a big difference in the heat flux, with the modified Woschni model having the highest heat flux among these models. This could be due to the use of a scaling factor in all models. When the scaling factor was the same for all models, the Hohenberg model had the highest heat flux. This is because the model is very sensitive to the temperature exponent under normal operating conditions. Therefore, correct tuning of constants is necessary before using the Woschni and Hohenberg models in a diesel HCCI engine simulation. The characteristic velocity scale is also important for predicting the heat loss because it has a direct impact on the heat flux. The study found that a modified Woschni correlation produced a more accurate result than the other two models and can be used for further analysis of a diesel HCCI engine.

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