Improving combustion chamber heat transfer correlation of an HCCI engine in order to achieve a more accurate thermodynamic model

A Qasemian¹,³ and M Rezaei²

¹ School of Automotive Engineering, University of Science & Technology, Tehran, Iran.
² Faculty of Technical Engineering Department of Mechanic, Islamic Azad University, Tehran North Branch, Iran
³ Tehran, Iran, Qasemian@iust.ac.ir

Abstract. An appropriate heat transfer rate prediction for an internal combustion engine is important from many perspectives. This study investigates the appropriate coefficients of heat transfer correlation and provides a new method for calculating the convective heat transfer coefficient of combustion chamber walls of an HCCI engine. Therefore, a thermodynamic code including the combustion and heat transfer processes, which are coupled with an optimization algorithm, is used to estimate P-θ behavior of an HCCI engine. Double-Wiebe function and Woschni correlations are applied for combustion and heat transfer respectively in a single-zone model. The results show that the use of heat transfer correlation without improvement in coefficients and exponents for different engines, leads to significant errors in the prediction of in-cylinder pressure. Comparison of computational results with the experimental data shows that original Woschni correlation in the single-zone model cannot predict in-cylinder pressure appropriately. Modifications made in this paper resulted in a change of more than 40% in some coefficients of the existing heat transfer correlation, to provide accurate prediction of the engine thermodynamic behavior of an HCCI engine.

1. Introduction
The homogeneous charge compression ignition (HCCI) engine is a new mode of internal combustion engine. The HCCI process essentially involves a premixed fuel/air combination at equivalence ratios that are generally lean. In this type of engine, combustion is controlled by heat released from chemical reactions and heat transferred from the in-cylinder charge to the cylinder walls.

The heat transfer from the in-cylinder charge to the cylinder walls is one of the most important tasks in HCCI simulations. There is no direct way to control the start of the combustion process in an HCCI engine and it influences the in-cylinder pressure and temperature, the fuel consumption and pollutants [1].
Due to the importance of heat transfer in the simulation of internal combustion engines, some correlations were developed for calculating convective heat transfer from in-cylinder gas to the wall in
compression ignition (CI) and spark ignition (SI) engines. Woschni [2], Annand [3], and Hohenberg [4] are some of these correlations.

Chang et al. [1] improved the accuracy of the Woschni correlation for an HCCI engine. They used height of combustion chamber as characteristic length and presented a new estimate for the coefficient $C_2$ and the temperature exponent in a Woschni correlation. Results showed that new optimized correlation could be useful for calculating convective heat transfer of a gasoline HCCI engine. Soyhan et al. [5] in 2008 studied different heat transfer correlations for the HCCI engines with a single-zone modelling. They examined the difference between heat transfer correlation and showed that there are significant differences between the correlations. Hensel et al. [6] in 2009 developed a new model for calculation of heat transfer to the combustion chamber walls. They investigated the heat loss in two different HCCI single cylinder engines. This model is well-manageable and the heat loss in the HCCI mode is more precise than the previous models. The effects of deposits and their thickness on heat transfer were considered in this study.

Multi zone models are among the most used models for simulating internal combustion engines. Multi zone models can predict engine combustion, performance and emission characteristics accurately; meanwhile, the run time is kept low. A new multi zone model was proposed by Asanis and Fiveland [7]. Neshat et al. [8] in 2015 proposed a new multi-zone model for simulating the HCCI engines. they offered a new relation for calculation of convective heat transfer from in-cylinder charge to combustion chamber walls of HCCI engines. By comparing the correlation, they concluded that Annand and Hohenberg correlations computed convective heat transfer coefficient higher than other correlations which caused incomplete combustion, while Chang and Woschni correlations over-predicted in-cylinder peak pressure slightly. Fathi et al. [9] in 2017 developed single zone and multi zone modeling for DI-HCCI engines. The lack of an efficient heat transfer correlation for such engines was mentioned in this study.

Regarding the weakness in the heat transfer correlation of HCCI engines where mentioned above, this paper uses a coupled thermodynamic, combustion, and heat transfer model to modify combustion chamber of HCCI engine to provide a more accurate prediction of these kind of engine performance.

2. Methodology

The simplest approach in engine modeling is to treat the cylinder contents as a single zone. The single-zone model views the burned and unburned gases, residual gases, and unburned hydrocarbons within the cylinder as a single, ideal gas with uniform pressure. In single-zone models, the single ideal gas is considered to be air.

Single-zone models typically use the Wiebe function to represent the chemical, or gross energy, release as a function of crank angle.

2.1. Governing equations

In this model our first step is to derive cylinder pressure as a function of crank angle using the first law of thermodynamics and ideal gas model. The ideal gas law shown is the basis of the computer modelling. Deriving equation (1) to $d\theta$ and then rewriting for $\frac{dp}{d\theta}$, equation (2) and (3) are obtained.

\[ PV = mRT \] (1)
The differential energy equation obtained from the first law of the thermodynamics for a closed system is given by Equation (4). Having Equation (5) for $\delta W$, Equation (6) for $dU$ and Equation (7) achieved by ideal gas law.

\[
\frac{dP}{d\theta} V + P \frac{dV}{d\theta} = m R \frac{dT}{d\theta} \tag{2}
\]

\[
\frac{dP}{d\theta} = \left( -\frac{P}{V} \right) \frac{dV}{d\theta} + \left( \frac{P}{T} \right) \frac{dT}{d\theta} \tag{3}
\]

Equation (4) can be written as Equation (9) for solving for the pressure, $P$ [10]:

\[
\frac{dP}{d\theta} = \left( -\frac{\gamma P}{V} \right) \frac{dV}{d\theta} + \left( \frac{\gamma - 1}{V} \right) \frac{dQ}{d\theta} \tag{9}
\]

Equation (9) is an implicit ODE which is solved numerically by a 4th-order Runge-Kutta numerical method. In Equation (9), combustion chamber instantaneous volume and its derivative is needed which are available in relevant references [10]. In addition to $V$, $\frac{dQ}{d\theta}$ that is given in Equation (9), can be defined as Equation (10):

\[
\frac{dQ}{d\theta} = LHV \left( \frac{dX_b}{d\theta} \right) - \left( \frac{dQ_w}{d\theta} \right) \tag{10}
\]

In calculating, $\frac{dQ_w}{d\theta}$ that shown by Equation (10) is the combustion chamber gas heat transfer to the wall for a crank angle of $d\theta$.

\[
\frac{dQ_w}{d\theta} = h_g A_w (T_g - T_w) \tag{11}
\]

In these equations, two parameters that play critical roles in predicting engine thermodynamic behavior are $X_b$ and $h_g$ shown in Equations (10) and (11) respectively. $X_b$ is double-Wiebe function and $h_g$ is combustion chamber HTC.

### 2.2. Burning rate, $X_b$

To simulate the combustion, we use the burning rate concept that explains the combustion process. The slower combustion is commonly modeled with a multi-zone approach (usually 2 or 3 zones) but it has been found that wall effects could be accommodated, without introducing a separate wall zone, by using a double-Wiebe function combustion model in which a fraction of the fuel (representing the wall region) burns at a reduced rate [11]. In an HCCI engine, double-Wiebe function defined by Equation (12) is utilized for this purpose.
\[ x_b = (1 - \alpha_{\text{wall}}) \left\{ 1 - \exp \left( -a \left( \frac{\theta - \theta_0}{\Delta \theta} \right)^{m+1} \right) \right\} + \alpha_{\text{wall}} \left\{ 1 - \exp \left( -a \left( \frac{\theta - \theta_0}{k_{\text{wall}} \Delta \theta} \right)^{m+1} \right) \right\} \]  \hspace{1cm} (12)

In this equation, the coefficient \( \alpha_{\text{wall}} \) shows the fraction of the mixture which is slowly burned in the combustion region and \( k_{\text{wall}} \) shows the ratio of the slow combustion duration to the standard combustion. The estimated value of these parameters for the HCCI engines is equal to 0.155 and 10, respectively [12]. The constant, \( \alpha \), essentially duplicates the role of the burn duration, \( \Delta h \). \( m \) is an adjustable parameter that fixes the shape of the combustion progress curve.

The easiest way to determine the ignition timing is the point that the value of \( \theta_0 \) become equal to the starting time of the combustion (i.e., \( \theta_0 = \theta_{\text{spark}} \)). However, considering the fact that \( \theta_0 \) as an adjustable parameter can be matched with the measured pressures, the starting time of combustion is considered a little later than \( \theta_0 \). This equation is briefly described as Equation (13)

\[ \theta_0 = \theta_{50} - \Delta \theta_{10-90} \frac{\ln(2)^{1/m+1}}{a_{10-90}} \]  \hspace{1cm} (13)

where, \( \theta_{50} \) is 50% burn time and \( \Delta \theta \) are adjustable constant that determine the combustion duration [12]. Figure (1) demonstrate standard Wiebe function and the double-Wiebe function for different \( m \).

![Figure 1. Wiebe function with different m values [12]](image)

2.3. Combustion chamber heat transfer coefficient, \( h_g \)

There are some models to estimate the combustion chamber heat transfer coefficient, \( h_g \) including Anand, Woschni, Eichelberg, Hohenberg, etc. In this study, the Woschni model is considered due to its inclusiveness and also the physics by which this model was proposed at the first time.

The original Woschni heat transfer correlation is given as Equation (14):

\[ h_g(\theta) = \alpha_s P(\theta)^{0.8} w(\theta)^{0.8} B^{-0.2} T(\theta)^{-0.55} \]  \hspace{1cm} (14)

where \( \alpha_s \) is a special coefficient used for tuning the correlation and specific engine geometry, \( B \) is bore, \( P \) and \( T \) are the instantaneous cylinder pressure and gas temperature respectively and \( w \) is defined as Equation (15)

\[ w = c_1 s_p + c_2 \frac{V_r T_r}{P_r V_r} (P - P_m) \]  \hspace{1cm} (15)
In this equation, \(C_1\) and \(C_2\) are the constants coefficients that can be changed for different engines. \(V_r\), \(T_r\), and \(P_r\) are volume, temperature and pressure at reference point. \(P_m\) is the motored pressure and \(V_d\) is the swept volume (m\(^3\)).

Equation (14), has been derived for CI engines [10] at the first time [Woschni]. Later, Chang [5] in Equation (16) modified original Woschni correlation for HCCI engines.

\[
h_g(0) = \alpha_s P(0)^{0.8} w(0)^{0.81} - 0.2 T(0)^{-0.73} \tag{16}
\]

As mentioned, in this correlation characteristic length and the temperature exponent have been improved. Where \(L\) is instantaneous chamber height (m), and the characteristic velocity is tuned as Equation (17).

\[
w = c_1 s_p + \frac{c_2 V_d T_r}{6 P_r V_T (P - P_m)} \tag{15}
\]

In this equation, \(C_1\) and \(C_2\) are constants and their values are equal to 6.18 and 0.0 for gas exchange process, 2.28 and 0.0 for compression process and 2.28 and 0.00324 for combustion and expansion processes.

Theoretical calculation and comparison with experimental data, as given in this study, shows that this modification cannot provide sufficient accuracy. Hence, this study in a thermodynamic model in which double-Wiebe function and original Woschni heat transfer are coupled, all coefficients and constants are considered to be corrected. For this purpose, the genetic algorithm (GA) method is used to minimize the errors of theoretical calculation in comparison with experimental values.

2.4. Optimization Algorithm

In this research, the genetic algorithm is used as an optimization algorithm for finding the most accurate constants and coefficients of an HCCI engine thermodynamic and heat transfer correlations. Genetic algorithms are commonly used to generate high-quality solutions to optimization and search problems by relying on bio-inspired operators such as mutation, crossover and selection [13].

Minimizing \(\varphi\), given by equation (16) is defined as the objective function in this research.

\[
\varphi = (Nump - Expo) \tag{16}
\]

The coefficients and exponents which are represented with the names of \(X_1\) to \(X_{10}\) in Equation (17) and (18) are the variables evaluated, (with the upper and lower bounds of 100%) in the genetic algorithm.

\[
h_g = X_8 (P X_1 w X_2 B X_3 T X_1) \quad w = X_6 s_p + \frac{X_7 (V_d T_r)}{P_r V_T (P - P_m)} \tag{17}
\]

\[
x_b = (1 - X_{10}) \left(1 - \exp \left(-X_8 \left(\frac{\theta - \theta_0}{\Delta \theta}\right)^{X_9+1}\right)\right) + X_{10} \left(1 - \exp \left(-X_9 \left(\frac{\theta - \theta_0}{X_{11} \Delta \theta}\right)^{X_8+1}\right)\right) \tag{18}
\]

In summary, Equations (17) and (18) help to calculate new results for simulation, which are explained in the next section.

3. Results and Discussion

3.1. Validation
To validate the present model, HCCI engine experimental results related to reference [6] are used. The characteristics of the HCCI single-cylinder engine used in this research are presented in Table 1.

**Table 1. Characteristics of Ricardo Hydra engine [5]**

| Parameters                  | Value | Unit |
|-----------------------------|-------|------|
| Bore                        | 86    | mm   |
| Stroke                      | 86    | mm   |
| Connection rod              | 143.5 | mm   |
| Compression ratio           | 14.04 | -    |
| Inlet valve diameter        | 32    | mm   |
| Number of valves            | 4     | -    |
| Inlet valve opening (IVO)   | 340   | CAD  |
| Inlet valve closing (IVC)   | 612   | CAD  |
| Exhaust valve opening (EVO) | 120   | CAD  |
| Exhaust valve closing (EVC) | 332   | CAD  |

The fuel was injected into the inlet port when the piston was in the TDC and located behind the intake valves closing.

By adjusting the amount of the fuel injection, the mixture strength is the constant value of 3.5. The intake temperature, intake pressure and the engine speed all held constants and they are 250 °C, 1 bar and 1200 rpm, respectively. Lubricant and coolant temperatures are both maintained at 90 °C [10].

As demonstrated in Figure 2, consistency of the obtained results by default model and experimental results seems inadequate. The error is more evident in expansion stroke, which has an average of 13 percent.

![Figure 2](image.png)

**Figure 2.** In-cylinder pressure vs. crank angle: comparison of experimental and original models
3.2. Corrected result

New optimized coefficients and constants in the thermodynamic model lead to more accurate prediction of HCCI engine pressure values shown in Figure 3. These new parameters have reduced the average error from 13% to 5%.

![Figure 3. In-cylinder pressure vs. crank angle- comparison of experimental, original model and optimized model](image)

Table (2) shows the values of $X_1$ to $X_{10}$ constants and coefficients in the default and optimized model.

| Parameters | Original model | Optimized model | Difference percentage |
|------------|----------------|-----------------|-----------------------|
| $X_1$      | 0.8            | 0.69            | 13                    |
| $X_2$      | 0.8            | 0.54            | 32                    |
| $X_3$      | -0.2           | -0.13           | 35                    |
| $X_4$      | -0.55          | -0.146          | 73                    |
| $X_5$      | 0.013          | 0.0237          | 82                    |
| $X_6$      | 2.28           | 2.160           | 5                     |
| $X_7$      | $3.24 \times 10^{-3}$ | $3.047 \times 10^{-3}$ | 6                  |
| $X_8$      | 1.5            | 1.405           | 6.3                   |
| $X_9$      | 0.99           | 1.25            | 26                    |
| $X_{10}$   | 0.155          | 0.155           | 0                     |
| $X_{11}$   | 10             | 10              | 0                     |
By these new parameters, burning rate does not show any significant change from its initial values as shown in Figure 4. This was predictable by little change of parameters $X_7$ to $X_{10}$ given in Table 2.

![Figure 4. Mass fraction burned vs. crank angle: original double-Wiebe function and optimized model](image)

With large m values, the combustion is very slow to start. In this study, by correcting the double-Wiebe function coefficients, the optimized m value is smaller (shown in Figure 4). This means the starting time of combustion is a bit faster.

On the other hand, as shown in Table 2, parameters $X_1$ to $X_5$ related to heat transfer show considerable changes after modification. The most change is related to parameter $X_5$ which is 82%. $X_5$ is the same as $\alpha$ scaling which has been studied in previous research. Other parameter that show great variation is $X_4$ which is temperature power. $X_4$ represents a percentage increase of 73% from its original value. The least change is related to the power of pressure, which shows 13% variation from its default value. These significant changes in the constants and coefficients of the original Woschni correlation lead to great differences between HCCI combustion chamber HTCs, demonstrated in Figure 5. As shown in this figure, optimized parameters result in more than 400% increase in HTC around the peak values.

![Figure 5. Variation of heat transfer coefficient vs. crank angle: original Woschni model and optimized mode](image)
The new HTC shown in Figure 5 indicates that the heat losses of an HCCI engine combustion chamber are much higher than the heat transfer model predicted in Woschni’s original correlation.

Finally, regarding all issues discussed above, this paper proposes a corrected correlation as Equation (19) to calculate the heat transfer coefficient of an HCCI combustion chamber.

\[ h_f(\theta) = 0.0237 P(\theta)^{0.69} w(\theta)^{0.54} B^{-0.13} T(\theta)^{-0.146} \] (19)

4. Conclusions

In this study, a theoretical formulation for calculating thermodynamic behavior of an HCCI engine was developed. The main purpose of this study was to investigate and improve the accuracy of an HCCI engine combustion chamber heat transfer coefficient. To achieve this goal, double-Wiebe function for combustion modeling and Woschni heat transfer correlation were coupled and optimized. Ten parameters existing in the correlations were considered as new variables. These new variables were corrected by GA optimization method. In the optimization process, minimizing the error between numerical results and experimental ones was regarded as the objective function. The results can be summarized as the following:

- Constants and coefficients related to heat transfer correlation showed significant variations up to 73%.
- The obtained results clearly showed that constants and coefficients related to the double-Wiebe function didn’t need any considerable correction, due to small changes.
- New corrected heat transfer correlation led to more than 400% increase in combustion chamber heat transfer coefficient of HCCI engines.
- All corrections made in the correlations, especially the heat transfer correlation which improved combustion chamber HTC, resulted in more precise prediction of engine P-\( \theta \). By this correction, the average error of numerical calculation reduced from 13% to 5%.

References

[1] J. Chang, O. Guralp, Z. Filipi, D. Assanis, New Heat Transfer Correlation for An HCCI Engine Derived From Measurements of Instantaneous Surface Heat Flux, [SAE paper 2004-01-2996].

[2] G. Woschni, A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in the Internal Combustion Engine; [SAE Paper 670931].

[3] W. J. D. Annand and T. H. Ma, Instantaneous Heat Transfer Rates to the Cylinder Head Surface of a Small Compression-Ignition Engine, Proc. Instn. Mech. Engrs., 1970-1971; 185: 976-987.

[4] G. F. Hohenberg, Advanced Approaches for Heat Transfer Calculations; [SAE Paper 790825].

[5] H. S. Soyhan, H. Yasar, et al, Evaluation of heat transfer correlations for HCCI engine modelling HAL, 2010.

[6] S. Hensel, F. Sarikoc, et al, a new model to describe the heat transfer in HCCI gasoline engines. SAE Int J Engines 2009; 2:33–47.
[7] S. Fivland, D. Assanis, A Four-Stroke Homogeneous Charge Compression Ignition simulation for combustion and Performance Studies, [SAE Paper, 2000].

[8] E. Neshat, and R.K. Saray, Effect of different heat transfer models on HCCI engine simulation Energy Conversion and Management, 2014. 88: p. 1-1,2014

[9] M. Fathi, O. Jahanian, S. Wang & B. Somers, Stand-alone single and multi-zone modeling of direct injection homogeneous charge compression ignition (DI-HCCI) combustion engines, Elsevier, 2017

[10] J. Heywood, Internal Combustion Engine Fundamentals. Tata: McGraw Hill Education, 2011.

[11] J. I. Ghojel, Review of the development and applications of the Wiebe function: A tribute to the contribution of Ivan Wiebe to engine research, International Journal of Engine Research 2010 11: 297

[12] H. Yasar, H. S. Soyhan, et al, Double-Wiebe function: An approach for single-zone HCCI engine modeling, Elsevier, 2008

[13] X. Yang, Computational Optimization, Methods and Algorithms. January 2011.