Amirkabir Univ. of Technology
Aerospace Engineering Dept.

The Third Fuel & Combustion Conference of IRAN

Tehran - IRAN Feb. 2010

Iranian Combustion Institue

FCCI2010-3156

MODIFIED FIRST LAW APPARENT HEAT RELEASE MODEL IN HCCI ENGINES

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ABSTRACT Homogeneous Charge Compression Ignition (HCCI) combustion has high heat release rate, short combustion duration and no evidence of flame propagation. In HCCI engines, there is no direct control method for the time of auto-ignition. Combustion timing control should be done in order to make heat release process take place at the appropriate time in the engine cycle. Heat release analysis is a diagnostic tool, which aids engine experimenters. It facilitates the endeavors being conducted in obtaining a control method by investigating heat release rate and cumulative heat release. In this study, a new heat release model based on the first law of thermodynamics accompanying with a temperature solver will be developed and assessed. The model was applied in four test conditions with different operating conditions and a variety of fuel compositions, including i-octane, n-heptane, pure natural gas (NG), and at last, a dual fueled case of NG and n-heptane. Results of this work indicate that utilizing the modified first law heat release model together with a solver for temperature correction will guarantee obtaining a well-behaved and accurate apparent heat release trend and magnitude in HCCI engines.

Keywords Apparent Heat release, HCCI, Specific heat ratio, Temperature correction

INTRODUCTION

In-cylinder NOx reduction methods are being widely studied. HCCI combustion mode proposed by Onishi et al. [1979] is a reliable method that has been found to produce ultra low NOx levels and near zero soot emissions; meanwhile, providing equal or greater fuel conversion efficiencies compared to that of conventional DI diesel combustion [Duret 2004, Sjoberg 2004, Hampson 2005]. The advantages of HCCI combustion are commonly associated with its nature being a spontaneous multi-site combustion of a highly diluted premixed fuel-air mixture which has high heat release rate (HRR) and no evidence of flame propagation [Hampson 2005, Hosseini 2006]. The high efficiency is due to the ability of operating with high compression ratios, lack of throttling losses at part load, lean combustion, and close to constant volume ideal Otto cycle heat release. There are some deficiencies intrinsic to HCCI combustion which should be overcome [Hampson 2005, Hosseini 2006]: the lack of any direct control method for combustion timing; high levels of HC and CO emissions; obtaining an appropriate fuelling rate for achieving high engine.

Since achieving HCCI combustion is generally difficult, it seems that heat release analysis is required for a manageable HCCI combustion as it relies on auto-ignition. Identifying early stages of heat release, timing of the main heat release, and maximum rate of heat release are necessary for a successful control strategy for HCCI combustion engine. Due to these facts and other benefits of heat release analysis [Heywood 1988, Gatowski 1984, Brunt 1999, Sastry 1994, Egnell 2000, Asad 2008], development of a suitable model for predicting apparent heat release, being able to be applied easily while eliminating erroneous assumptions, is quite necessary.

To date, numerous researchers have studied heat release analysis in both SI and CI engines. Rassweiler and Withrow [1938] did one of the earliest simple attempts in the 1930's. R-W method was a simple but efficient method based on correlation between pressure trace and burnt/unburnt fraction of air/fuel mixture using combustion chamber pictures. Krieger and Borman [1966] presented heat release models for both SI and CI engines. In addition, their work included the effect of dissociation of the product species. Their models as stated by Gatowski et al. [1984] strive for accuracy in representing the thermodynamic properties of the cylinder charge and involve substantial computations. Gatowski et al. [1984] presented a model as they claimed being the first to give a full description of a heat release model, which is simple in approach and accounts for all major loss mechanisms while keeping the calculation method simple, as a single zone heat release analysis procedure. Other researchers also developed this kind of modeling, but their works were to optimize existing models in terms of, for example, the correlations used. These correlations were namely correlations for heat transfer, specific heat ratio, etc. For instance, Chun and Heywood [1987] argued that better results could be achieved if the assumption of linearity with temperature for the ratio of specific heats was studied in more details.

In the current study, due to the lack of a reliable work on heat release analysis in HCCI engines, the focus is on investigating the applicability of simplified first law heat release (SFLHR) model in interpreting HCCI combustion. Due to the simplifying assumptions, this model cannot well and fully predict heat release trend and magnitude in such engines. Thus, a modified first law heat release (MFLHR) model that puts aside erroneous assumptions together with a solver for temperature correction, which calculates the heat released from combustion more accurately, has been developed and will be presented.

EXPERIMENTAL SETUP

Experiments were conducted in University of Alberta engine research facility. All experiments were performed using a Waukesha CFR single cylinder research engine coupled to a DC motoring dynamometer. The basic engine specifications for the current study are shown in Table 1. The engine was maintained at constant speeds of 700 or 800 RPM and ran with an open throttle. The intake system included a 2.4 kW heater with a PID temperature controller to preheat intake air when required. Two port fuel injectors including one liquid fuel injector for diesel type fuel and a gaseous fuel injector for NG were installed a short distance upstream of the intake valve to ensure proper mixing. The lubricating oil was maintained at a constant temperature using a heater. A BEI rotary incremental encoder with a resolution of 0.1 CAD monitored engine rotational speed and coordinated the pressure trace with respect to crank position. Cylinder pressure was measured with a Kistler 6043A water-cooled pressure transducer in combination with a Kistler 507 charge amplifier. The pressure transducer was mounted in the cylinder wall close to the cylinder head. Experimental data were acquired using a personal computer running custom Labview software and using three high sampling rate NI PCI-MIO-16E1 data acquisition cards. The pressure trace signal was referenced to the intake pressure at the time of IVC. Proper digital filter was applied to the pressure trace signal rejecting the high frequency noise.

Table 1
Engine Specifications

parameter	specification
Engine model	Waukesha CFR
Engine type	Water cooled, single cylinder
Combustion chamber	Disk cylinder head, flat-top piston
(Bore× Stroke) × displacement	(82.6×114.3mm) × 612 cc

Four experimental conditions were tested. Normal heptane was added to NG in order to enhance the HCCI combustion process. Table 2 illustrates the CFR engine operating conditions used in these experiments. The coolant temperature for all cases was set to 100 centigrade degrees. To eliminate the effects of cyclic variations, the pressure traces of all cases were averaged over 100 consecutive cycles. Hence, these averaged cylinder pressure traces were utilized in calculations.

Table 2
CFR engine operating conditions for four considered cases

	Case 1	Case 2	Case 3	Case 4
Fuel	i-octane	n-heptane	NG	n-heptane + NG
Compression ratio	13.5:1	11.5:1	17.25:1	13.8:1
Speed (rpm)	700	700	800	800
PRF mass flow rate (mg/s)	78.5	79.9	0	36.4
NG mass flow rate (mg/s)	0	0	82.3	21.8
Air mass flow rate (g/s)	2.4	2.6	4.5	2.5

MATHEMATICAL TREATMENT

The SFLHR model is the result of applying first law of thermodynamics to the engine combustion chamber charge. This model was first fully developed by Gatowski et al. [1984]. The heat release model commonly used in the literature is:

$$\delta Q_{gross} = \frac{\gamma}{\gamma-1} pdV + \frac{1}{\gamma-1} Vdp + \delta Q_{ht} \tag{1}$$

Equation (1), gives the apparent gross heat release on the intervals, which is not an exact one. There are a number of assumptions in developing Equation (1):

1. The state of the cylinder contents is defined as average properties of the uniform charge.
2. The change in sensible internal energy is a function of mean charge temperature only.
3. The ideal gas law determines the mean charge temperature.
4. The specific gas constant is assumed constant and this assumption has its root in that the molecular weights of the reactants and products are nearly identical [Gatowski 1984].

This model cannot well and fully predict the accurate apparent cumulative gross heat release trend and magnitude in HCCI engines. To overcome this deficiency, the modified first law heat release (MFLHR) model accompanying with a solver for correction of temperature will be proposed and investigated. MFB is calculated from the model developed by Rassweiler and Withrow [1938]:

$$MFB_\theta = \sum_{i=IVC}^{\theta} \Delta p_{c,i} \Big/ \sum_{i=IVC}^{EEOC} \Delta p_{c,i} \tag{2}$$

Δp_c ,the corrected pressure rise due to combustion is:

$$\Delta p_{c,i} = \left[p_i - p_{i-1}(V_{i-1}/V_i)^n\right]\left(V_{i-1}/V_r\right) \tag{3}$$

The specific heat ratio depends on temperature and composition and to a lesser extent on pressure. Here in this study, the equilibrium combustion model of Olikara and Borman [1975] was fully incorporated with the model to evaluate the specific heat ratio and internal energy, using the thermodynamic data of JANAF table. The equilibrium combustion model was implemented by considering the products being composed of 11 species. Thus, the specific heat ratio model, which is used in MFLHR model, is a function of both temperature and composition.

In the present study, the well-known expression proposed by Woschni [1967] with modifications, which made it be appropriate for HCCI engines has been used [Filipi 2004], to evaluate convective heat transfer. In this work, the radiative heat loss has been ignored.

$$\delta Q_{ht} = h \times A \times (T - T_{wall}) \tag{4}$$

The convective heat transfer coefficient is approximated by:

$$h_c = 3.4 \times height^{-0.2} p^{0.8} T^{-0.73} S^{0.8} \tag{5}$$

where
height : effective height of the chamber which is equal to V/A [Filipi 2004], instead of bore which was used in the original Woschni expression
The characteristic velocity is obtained as follows:

$$S = C_1 S_p + C_2 \frac{V_d T_{IVC}}{p_{IVC} V_{IVC}}(p - p_m) \tag{6}$$

where
C_1 = 2.28
C_2 = 0 for compression and $5.4*10^{-4}$ for combustion and expansion
C_2 was modified to fit HCCI combustion engine characteristics. The MFLHR model is achieved by applying the energy conservation equation to the cylinder contents and not utilizing erroneous assumptions. The first law of thermodynamics for the cylinder charge during closed valve interval by ignoring mass leakages yields:

$$dU = -\delta W - \delta Q_{ht} \tag{7}$$

where, U is the absolute internal energy of the cylinder contents. By considering the in-cylinder charge to be a homogeneous mixture of reactants (denoted by the R index), products (denoted by P index), and recycled exhaust gases (denoted by the EGR index), which are supposed to be ideal gases:

$$m = m_R + m_P + m_{EGR} \tag{8}$$

$$dm_P = -dm_R \tag{9}$$

$$U = m_R\left(u_{s,R} + u_{f,R}\right) + m_P\left(u_{s,P} + u_{f,P}\right) + m_{EGR}\left(u_{s,EGR} + u_{f,EGR}\right) \tag{10}$$

By differentiating equation (10), the equation for internal energy change is obtained:

$$dU = \left(u_R - u_P\right)dm_R + m_R du_{s,R} + \left(m - m_{EGR} - m_R\right)du_{s,P} + m_{EGR} du_{s,EGR} \tag{11}$$

Substituting equation (11) and the work term into equation (7) yields:

$$\begin{aligned}&\left(u_{f,R} - u_{f,P}\right)dm_R + \left(u_{s,R} - u_{s,P}\right)dm_R + m_R du_{s,R} \\ &\quad + \left(m - m_{EGR} - m_R\right)du_{s,P} + m_{EGR} du_{s,EGR} = -pdV - \delta Q_{ht}\end{aligned} \tag{12}$$

The gross heat release for an incremental crank angle interval is:

$$\delta Q_{gross} = \left(u_{f,P} - u_{f,R}\right)dm_R \tag{13}$$

Substitution of equation (13) into equation (12) yields the MFLHR model:

$$dQ_{gross} = \left(u_{s,R} - u_{s,P}\right)dm_R + + m_R du_{s,R} + \left(m - m_{EGR} - m_R\right)du_{s,P} + m_{EGR} du_{s,EGR} + pdV + \delta Q_{ht} \tag{14}$$

m_R is the mass of reactants at any instant and equals to:

$$m_R = \left(1 - MFB\right)\left(m_{f,i} + m_{air,i}\right) \tag{15}$$

where $m_{f,i}$ and $m_{air,i}$ are the fuel and air mass at IVC, respectively. dm_R, is the change in mass of the reactant component due to combustion.

Here in this model, it is not only assumed the change in sensible internal energy being a function of temperature but also a function of composition, too. The difference between this model and the SFLHR model (equation (1)), is that in the SFLHR model it was first assumed that the change in the internal energy is a function of temperature only to obtain equation (1) to be the governing equation of SFLHR model. Then, for refining the results, it was assumed that the gamma term is a function of composition and temperature. By contrast, here the dependency of internal energy on composition and temperature was applied into the model itself.

Solver For Temperature Correction Using the ideal gas law for temperature calculation, the cumulative gross heat release trend will be at fault, even when utilizing MFLHR model. Investigating these errors, a solver was developed for the mean charge temperature. The internal energy of the homogeneous charge including reactants, i.e. fuel vapour and air, and products which were supposed to be composed of 11 species, namely, CO_2, H_2O, CO, N_2, O_2, H_2, OH, NO, O, H, N, according to the model of Olikara and Borman [1975], was evaluated using the thermodynamic data of JANAF table.

The correction of the temperature was achieved by solving the initial value problem of ordinary differential equation (ODE) of energy by the aid of fourth-order Runge-Kutta method. The approach was:

1. First, the energy equation should be rewritten to produce a function of temperature, species composition and time:

$$(u_R - u_P)\frac{dm_R}{dt} + m_R\frac{du_{s,R}}{dt} + (m - m_{EGR} - m_R)\frac{du_{s,P}}{dt} + m_{EGR}\frac{du_{s,EGR}}{dt} + p\frac{dV}{dt} + hA(T - T_{wall}) = 0 \quad (16)$$

By replacing the thermodynamic properties and specific heats of each species with polynomial functions fitted from the JANAF table,

$$\bar{c}_{v_i} = Ru\left(a_1 - 1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4\right) \quad (17)$$

$$\bar{u}_i = Ru\left[(a_1 - 1)T + \frac{a_2}{2}T^2 + \frac{a_3}{3}T^3 + \frac{a_4}{4}T^4 + \frac{a_5}{5}T^5 + a_6\right] \quad (18)$$

And the ODE of energy equation, by applying the aforementioned replacement and arrangement, will take the following final form:

$$\frac{dT}{dt} = A_5T^5 + A_4T^4 + A_3T^3 + A_2T^2 + A_1T + A_6 \quad (19)$$

Where, A_1 to A_6 are instantaneous constants of the equation, which are themselves functions of temperature, pressure and species mole fractions at any instant, obtained from arrangement of polynomial coefficients of overall 14 species together with their mole fractions and production rates.

2. This produced equation was used to determine the corrected temperature by fourth-order Runge-Kutta method:

$$\frac{dT}{dt} = \mathrm{fcn}(t, T) \quad \& \quad T_0 = T_{IVC} \quad (20)$$

Where the step size equals to:

$$h = {}^{0.1}\!/_{6N} \quad (21)$$

This procedure was applied to the model from SOC to EVO. It can be seen from the results, that this corrected temperature gives acceptable results. It is also worth mentioning here, that the CPU time required for the model to be executed was less than 60 seconds.

RESULTS AND DISCUSSION

Figure 1a shows the HRR and Figure 2a illustrates the corresponding cumulative gross heat release for case 1. It can be seen from these figures that applying the traditional SFLHR model to HCCI engines, which have short combustion durations approximately centered at TDC, produces large errors. It is well known that the gross HRR should not be negative after the completion of combustion, and consequently the cumulative gross heat release should not decrease following the end of combustion. However, as can be seen in these figures, there are negative heat release gradients following the end of combustion, not only when applying SFLHR model but also in the case of utilizing MFLHR model without temperature correction, which is obviously wrong. These figures indicate that there is no evidence of negative heat release gradient after the completion of combustion when applying MFLHR model together with the temperature correction solver. Thus, it is guaranteed that applying the developed model to HCCI engines, which have very short combustion durations, results in the correct trend and magnitude in the heat release diagrams for this case.

In Figure 1b, the HRR and in Figure 2b, the corresponding cumulative gross heat release for case 2, are shown. The two-phase nature of n-heptane combustion can be seen in these diagrams. Again, it can be seen that the correct trend can be obtained, only when the MFLHR model accompanying with the temperature correction procedure is used. These figures and also Figures 1a and 2a show that applying the wrong model for apparent heat release gives erroneous results not only in diagrams trend, but also in the low magnitude of peak HRR and cumulative heat release in these cases.

Figures 1c and 2c show the HRR and cumulative gross heat release for case 3, respectively. The above-mentioned results can be seen in these two figures, too. But, in this case, the magnitude of peak HRR and cumulative heat release has been lowered due to applying temperature correction. In addition, it can be seen that applying MFLHR model together with the temperature correction solver has diminished the negative temperature combustion trend, which should not be seen in the combustion of NG.

The HRR and cumulative heat release diagrams are shown in Figures 1d and 2d, respectively, for the fourth case. Again, it is obvious that MFLHR model when accompanied with the temperature correction procedure, gives acceptable results, both in terms of shape and magnitude.

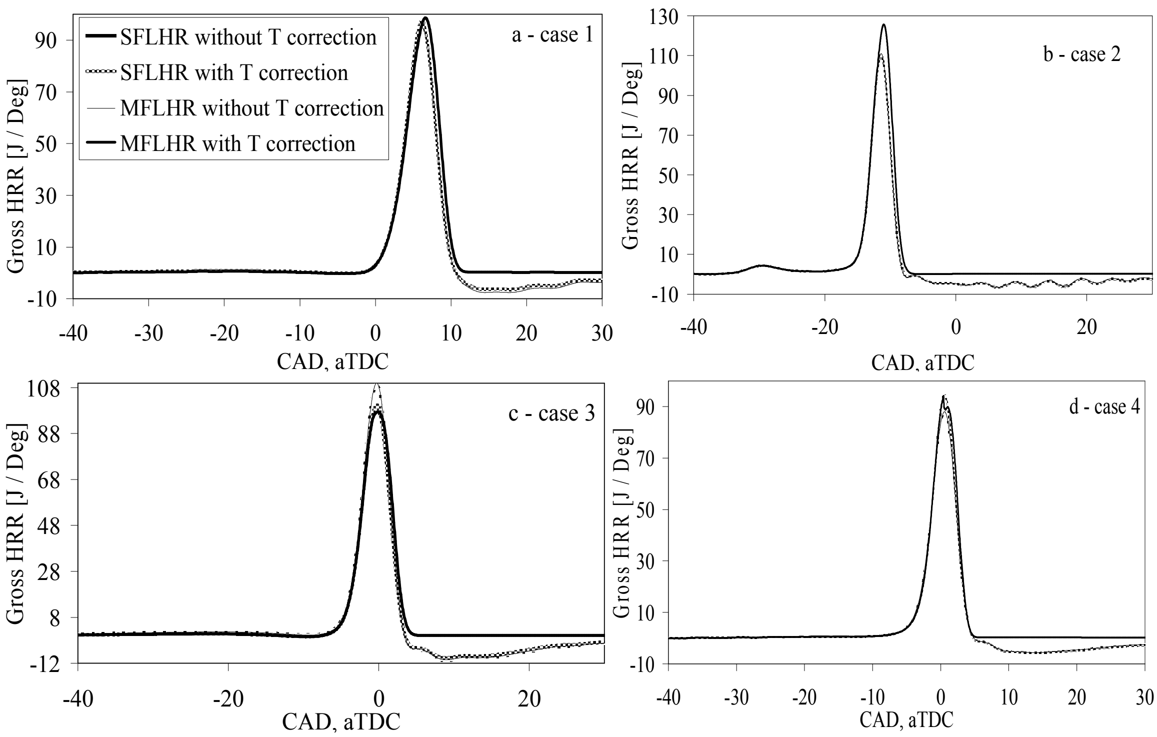

Figure 1. HRR obtained from different models for different cases

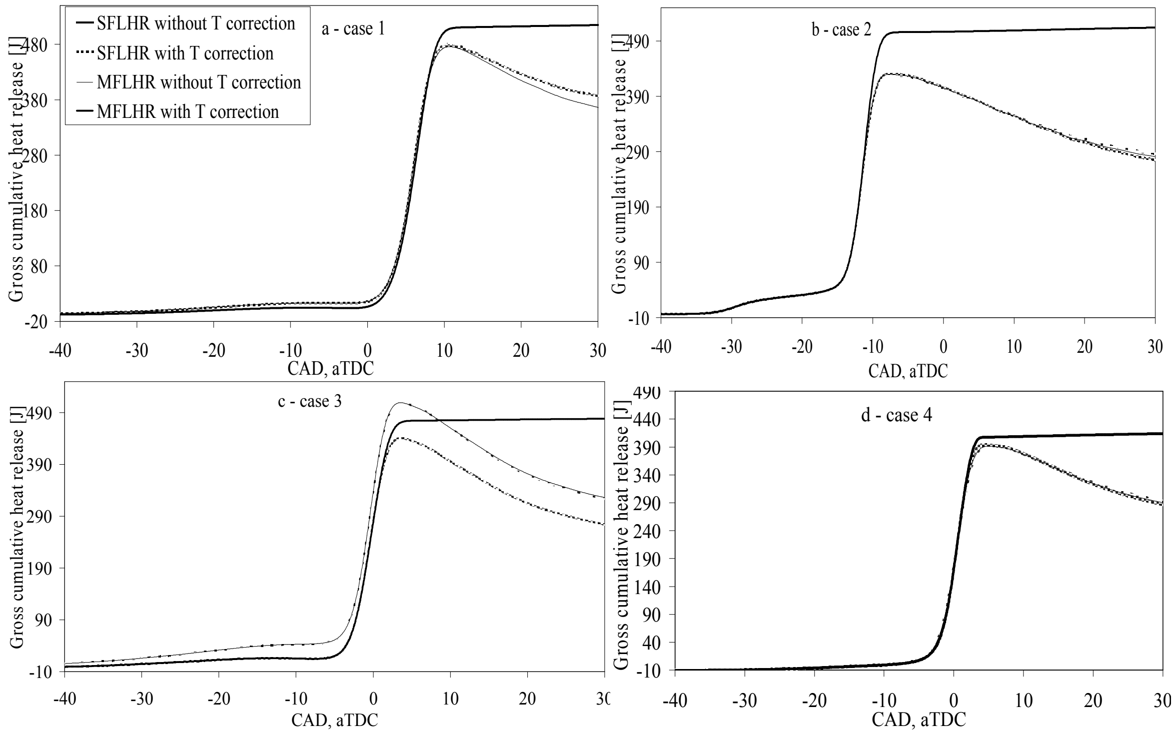

Figure 2. Gross cumulative heat release obtained from different models for different cases

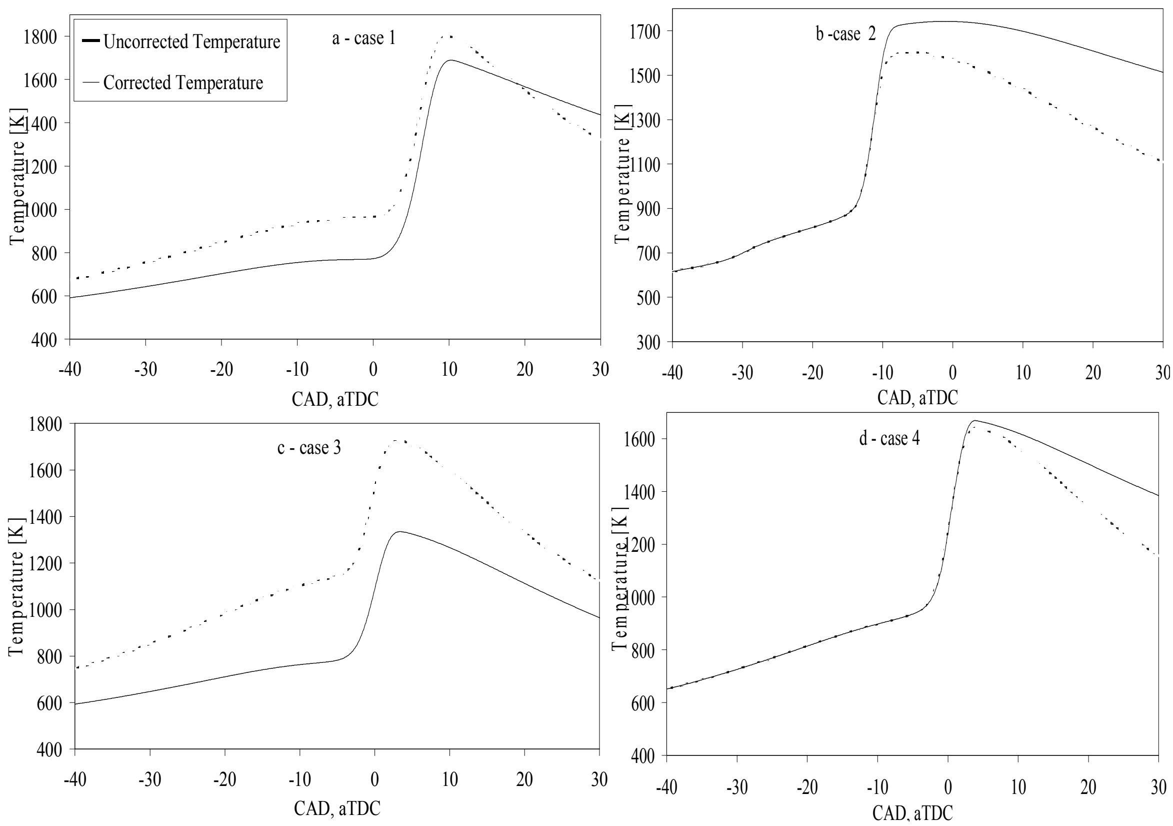

Figure 3. The comparison between temperatures calculated from ideal gas law and temperature correction procedure for different cases

The comparison between mean charge temperatures calculated from ideal gas law and temperature correction procedure are demonstrated in Fig. 3. It can be seen that the correction procedure for temperature has smoothen the temperature diagram, lowered its peak temperature, and increased its post combustion temperature, for case 1. For cases 2 and 4, this procedure has increased both the peak and post combustion temperature. Applying temperature correction procedure has totally lowered the temperature for case 3.

CONCLUSIONS

In this study, the applicability and accuracy of traditional SFLHR model applied to HCCI engines have been investigated. To achieve this assessment, several specific heat ratio models proposed in the literature were applied to this model and the result of the most accurate, which is a function of temperature and composition, are shown in the results, and four cases were evaluated. Results show that this model cannot well and fully predict the accurate apparent cumulative gross heat release trend and magnitude. To overcome this deficiency, the MFLHR model accompanying with a solver for correction of temperature was proposed and investigated. The results from this model, for all the various working conditions and fuel compositions of evaluated cases, show good agreement with the concept that states there should not be any indication of negative gradient in gross heat release.

The results indicate that in HCCI engines, utilizing traditional SFLHR model results in erroneous results. However, applying MFLHR model together with temperature correction procedure ensures obtaining more accurate results.

ACKNOWLEDGMENT

The Iranian Fuel Consumption Organization (IFCO) financially supported this study, which is highly acknowledged. In addition, the authors wish to thank gratefully Professor M D Checkel, due to his ongoing scientific support, and providing the engine research facility of University of Alberta for the tests to be experimented.

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