ENERGY AND EXERGY ANALYSES OF HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINE

by

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In the present investigation, a single-cylinder, four-stroke cycle, TD43 engine has been used to evaluate the first and second laws of thermodynamics terms. To this aim, the first law analysis is done by using a thermo-kinetic model. The results show a good agreement with the experimental data. Also for the second law analysis, a developed in house computational code is applied. Behaviors of the results have a good accordance with the literature. The result show that an increase in the inlet charge temperature causes the maximum pressure, indicated work availability and entropy generation per cycle be reduced and the in-cylinder temperature, heat loss availability and total availability be increased. Also the results show that an increase in the engine speed causes the total availability be increased and the heat loss availability be decreased. When the engine speed increases, reduction in the duration of cycle evolution causes the reduction of heat transfer.

Key words: *availability, exergy, homogeneous chare compression ignition engine, irreversibility*

Introduction

It has been more than one century that the basic operation of gasoline and diesel engines has not been the subject of revolutionary changes. Environmental pollutions and energy limitations make us to replace old combustion method with those which fulfill our new concerns. A promising alternative to combustion in Otto and Diesel engines is the homogeneous charge compression ignition (HCCI) process which requests detailed attention [1]. This engine uses a lean premixed air/fuel mixture that is compressed with high compression ratio, resulting in simultaneous auto-ignition in the whole combustion chamber. Furthermore, theoretically the HCCI process eludes locally lean high temperature regions and rich low temperature regions compared to the combustion process for conventional diesel engine. HCCI is currently under widespread investigation due to its potential to lower NO_x and particulate emissions while maintaining high thermal efficiency [2, 3]. Since HCCI combustion is achieved through auto-ignition, the chemical kinetics of the fuel-air mixture plays a key role in determining various combustion characteristics (*e. g.* ignition start, burn duration). These effects impact the operating range in which HCCI combustion can be employed. The HCCI engine concept has superior potential for achieving high part load fuel conversion efficiency. This is due to the combination of small pumping losses, high compression ratio and short combustion period.

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Engine simulation is a very effective tool to approximate engine performance and improve it. First law analysis is a proper method to predict engine performance and influence of its various operative parameters [4]. On the other hand, it has long been understood that traditional first law analysis, which is needed for modeling the engine processes, often fails to give the engineer the best in sight into the engine's operation. In order to analyze engine performance, that is to evaluate the inefficiencies associated with the various processes, second law analysis must be applied [5, 6]. For the second law analysis, the key concept is "availability or exergy". The availability of a matter explains its potential to produce useful work. Unlike energy, availability can be destroyed, which is a result of some phenomena such as combustion, friction, mixing, throttling, *etc*. The destruction of availability is a source for insufficient use from fuel availability to produce useful mechanical work in an internal combustion engine. The reduction of irreversibilities can lead to better engine performance through a more efficient exploitation of fuel [7]. Many studies have been published in the past few decade (the majority during the last 20 years) concerning second law application to internal combustion engines. The first studies of internal combustion engines operation that included exergy balance in the calculations were around 1960, the works of Traupel [8] and Patterson and Van Wylen [9]. Flynn *et al*. [10], explained a new observation in internal combustion engine studies. They applied a method based on the second law of thermodynamics for engine analysis. A review paper written by Caton [11], explains previous studies of engine operation from the second law observation. Abassi *et al.* [12] analyzed influence of the inlet charge temperature on the second law balance under the various operative engine speeds in direct injection (DI) diesel engine.

The present work analyzes operation of an HCCI engine from a first and second-law analysis point of view. For this purpose, a single zone thermo-kinetic model has been used. Also for the second law analysis, a homemade computational code is developed. The second law terms such as indicated work availability, availability loss associated with the heat transfer to walls, combustion irreversibility, entropy generation per cycle are evaluated by this code.

Model description

In the present study, HCCI engine operation is analyzed from the first and second law of thermodynamics perspective and the various terms are evaluated. The first law analysis is done by using a single zone thermo-kinetic model. The combustion chamber of an HCCI engine is considered as a single thermodynamic zone with the assumption of a uniform thermodynamic state within the zone. It is assumed that all species in the zone can be treated as ideal gases and blow-by is negligible and mass of in-cylinder mixture is constant. Evaporation of fuel in the intake port and combustion chamber is also neglected and it is assumed that the entire mixture is in the gas phase. Furthermore, an average temperature of combustion chamber walls is used to consider the convective heat transfer between the zone and its surroundings. The first law analysis of the system is used to determine the variation of the thermodynamic state of the mixture as time passes. This results in the following equation to calculate the rate of change of the mixture temperature (T) [13]:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{-P\dfrac{\mathrm{d}V}{\mathrm{d}T} - \dfrac{\mathrm{d}Q_\mathrm{w}}{\mathrm{d}t} - \sum_i \dfrac{\mathrm{d}N_i}{\mathrm{d}t}\bar{h}_i + \mathrm{R_u}T\sum_i \dfrac{\mathrm{d}Ni}{\mathrm{d}t}}{\sum_i N_i \bar{c}_{\mathrm{p,i}} - N_{\mathrm{mix}}\mathrm{R_u}} \tag{1}$$

where P is the in-cylinder gas pressure and N_i and $c_{\mathrm{p,i}}$ are the number of moles and the molar specific heat of the specie, respectively. $\mathrm{R_u}$ is the universal gas constant, and V – the cylinder volume which is calculated at any crank angle from engine geometry by using crank-slider mechanism equations [4]. Q'_w is the heat excanged per unit time between the in-cylinder gas and the surrounding walls.

Q'_w is modeled using the Modified Woschni heat transfer correlation that is adopted for HCCI engines [14]:

$$Q'_w(t) = -h_c(t)A_s(T_g - T_w) \tag{2}$$

where A_s is the in-cylinder surface area, T_g and T_w are gas temperature and average wall temperature, respectively, and h_c is the convective heat transfer coefficient is given by:

$$h_c(t) = \alpha_{\text{scaling}} L(t)^{0.2} P(t)^{0.8} T(t)^{0.73} \omega(t)^{0.8} \tag{3}$$

$$\omega(t) = C_1 S_p + \frac{C_2}{6} \frac{V_d T_r}{P_r V_r} (p - P_{\text{mot}}) \tag{4}$$

where L is the instantaneous cylinder height, P and T are the gas temperature and pressure, respectively, ω is the local gas velocity, S_p – the average piston speed, T_r , P_r and V_r are temperature, pressure, and volume at the *IVC* moment, respectively, V_d is the displacement volume and P and P_{mot} are instantaneous pressure and the corresponding motoring pressure at the same firing condition. C_1 and C_2 are constant values and $\alpha_{scaling}$ is the scaling factor for different engine geometries [15].

The chemical kinetic mechanism consists of 155 species and 689 reactions for describing the combustion of arbitrary Iso-butane blends.

The availability of a system in a given thermodynamic state is defined as the maximum useful mechanical work that can be produced as the system is brought to thermal, mechanical, and chemical equilibrium with its environment through reversible processes [7]. Once the system is brought into equilibrium with the environment, no further work can be obtained. It is customary to divide the availability content of a system into two parts: the thermo-mechanical availability and the chemical availability. The chemical availability for a substance which is not present in the environment (*e. g.* fuel, sulfur, combustion products such as NO or OH, *etc.*) can be evaluated by considering an idealized reaction of the substance with other substances for which the chemical exergies are known [16]. For hydrocarbon fuels of the type C_zH_y, the chemical availability of the fuel can be expressed as follows [6]:

$$a_{\text{fch}} = LHV\left[1.04224 + 0.011925\frac{y}{z}\right] - \frac{0.042}{z} \tag{5}$$

where *LHV* is the fuel lower heating value. The thermo-mechanical availability can be determined using the following formula [17]:

$$A_{\text{th}} = (U - U_0) - P_0(V - V_0) - T_0(S - S_0) \tag{6}$$

The total availability of a closed system is defined as:

$$A = A_{\text{th}} + a_{\text{fch}} \tag{7}$$

Cylinder availability balance can be formulated as [12]:

$$\frac{\mathrm{d}A_{\text{cyl}}}{\mathrm{d}\Phi} = \frac{\dot{m}_{\text{in}} b_{\text{in}} - \dot{m}_{\text{out}} b_{\text{out}}}{N} - \frac{\mathrm{d}A_w}{\mathrm{d}\Phi} - \frac{\mathrm{d}A_l}{\mathrm{d}\Phi} + \frac{\mathrm{d}A_f}{\mathrm{d}\Phi} - \frac{\mathrm{d}I}{\mathrm{d}\Phi} \tag{8}$$

where $\dot{m}_{in}$ is the inlet mass flow from the inlet manifold, $\dot{m}_{out}$ – the outlet mass flow from the outlet manifold, and b represents flow availability as [12]:

$$b=(h-h_0)-T_0(S-S_0) \tag{9}$$

$\mathrm{d}A_\mathrm{w}/\mathrm{d}\Phi$ represents indicated work transfer. In fact it can to be known as value of output availability from the cylinder associated with the indicated work [12]:

$$\frac{\mathrm{d}A_\mathrm{w}}{\mathrm{d}\Phi}=(P_\mathrm{cyl}-P_0)\frac{\mathrm{d}V}{\mathrm{d}\Phi} \tag{10}$$

where $\mathrm{d}V/\mathrm{d}\Phi$ states the rate of change of cylinder volume based on crank angle degree and P_cyl – the instantaneous cylinder pressure that which are both computed by the first law analysis about the engine processes. P_0 represents the ambient pressure. $\mathrm{d}A_i/\mathrm{d}\Phi$ is the rate of availability loss associated with the heat transfer to the cylinder walls on the basis of crank angle degree. It can be given as [12]:

$$\frac{\mathrm{d}A_i}{\mathrm{d}\Phi}=\frac{\mathrm{d}Q_l}{\mathrm{d}\Phi}\left(1-\frac{T_0}{T_\mathrm{cyl}}\right) \tag{11}$$

$\mathrm{d}Q_\mathrm{l}/\mathrm{d}\Phi$ is the rate of the heat transfer to the cylinder walls on the basis of crank angle degree and T_cyl – the instantaneous temperature of the cylinder gasses, which are both available from the first law analysis. T_0 represents the ambient temperature. $\mathrm{d}A_\mathrm{f}/\mathrm{d}\Phi$ is the burned fuel availability based on crank angle degree which can be given as [12]:

$$\frac{\mathrm{d}A_\mathrm{f}}{\mathrm{d}\Phi}=\frac{\mathrm{d}m_\mathrm{fo}}{\mathrm{d}\Phi}a_\mathrm{fch} \tag{12}$$

S_gen is the entropy generation per a cycle which can be given as [12]:

$$S_\mathrm{gen}=(S_\mathrm{out}-S_\mathrm{in})+\frac{Q_\mathrm{loss}}{T_0}+\frac{I_\mathrm{total}}{T_0} \tag{13}$$

where S is the gas entropy, Q_loss – the heat transfer to the cylinder walls, I_total – the total irreversibility, and T_0 – the ambient temperature.

Table 1. Engine characteristics [18, 19]

Cylinder bore	95 mm
Stroke	82 mm
Displacement	582 cm^3
Connecting rod	156 mm
Compression ratio	5:1-18:1

Results and discussion

The specifications of the engine used are given in tab. 1. A single-cylinder, four-stroke cycle, TD43 fuelled with Iso-butane, was used as prototype engine because of its variable compression ratio mechanism and high durability. Further detailed description of the experimental apparatuses has also been reported by Ebrahimi [18] and Ebrahimi and Desmet [19].

To show the model validation from the first law perspective, diagram of the cylinder pressure is compared with the experimental data [18] (fig.1) and a good agreement is seen. Similar to all zero dimensional models, the pick cylinder pressure is higher than the experimental result. This is the main disadvantage of zero dimensional models that originate from considered uniform temperature and uniform composition of charge throughout the cylinder.

Although speed as one parameter for control ignition timing is not used in HCCI engine, its influence on start of ignition should be considered. In this part of our study, the engine speed varies from 600 rpm to 3500 rpm and its effects on the energy and exergy terms will be investigated. The calculations are carried out in conditions as: compression ratio of 18 and inlet charge temperature of 460 K.

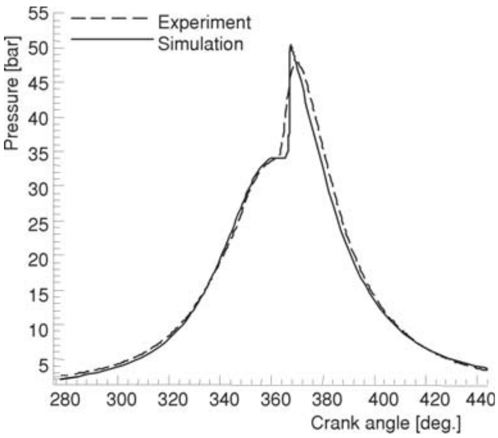

Figure 1. Model validation under engine speed 600 rpm and inlet temperature 313 K

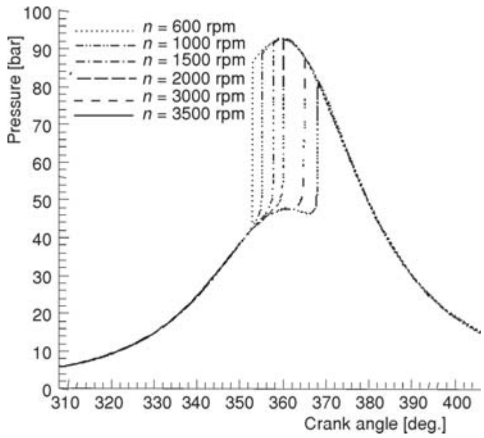

Figure 2. In-cylinder pressure under various engine speeds

Figure 2 shows the variations of the pressure as a function of crank angle in the various engine speeds. According to this figure, as the engine speed increased, the start of ignition is retarded. For example, in this case, the speed of 3000 rpm ignition starts after top dead center (TDC) that maximum cylinder pressure decreases. Engine speed reduction causes the mixture expose to high pressure and temperature for a longer duration, and to need less inlet temperature for creating auto- ignition.

Figure 3 reveals that an increase in the speed decreases the in-cylinder temperature. In low speeds, ignition happens quicker. If by fixing the other parameters, the speed increases more, so ignition starts with more delay and even there is a possibility that the ignition will not happen at all as can be seen in fig. 4. In this figure, the pressure has been compared at the three speeds of 2500, 4000, and 4700 rpm. According to this figure, at the speed of 4700 rpm, the mixture does not ignite anymore.

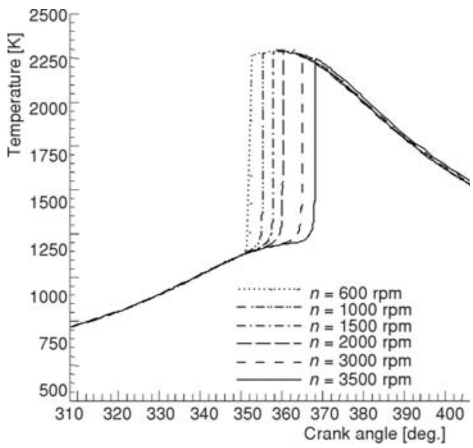

Figure 3. In-cylinder temperature under various engine speeds

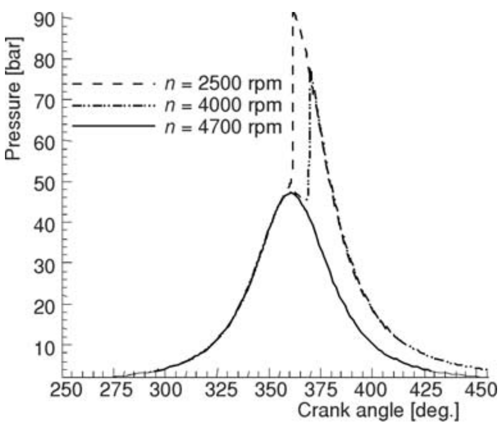

Figure 4. In-cylinder pressure under various engine speeds

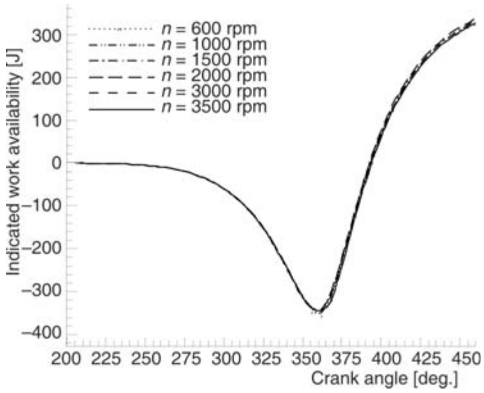

Figure 5. Indicated work availability under various engine speeds

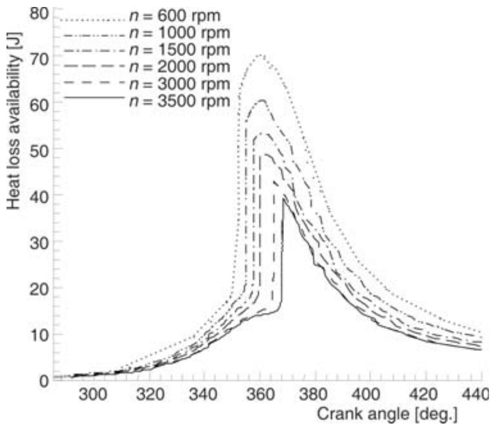

Figure 6. Heat loss availability under various engine speeds

Work exergy is defined as the availability of the system to do actual work on a changing control volume against its surroundings. As fig. 5 shows, by increasing engine speed, indicated work availability has a minor variations and first increases, and then by increasing engine speed to 2000 rpm, when ignition happens after TDC, indicated work availability decreases. Also transfer of exergy to the system via compression work is the reason for the negative value of the curve during compression.

Figure 6 illustrates the variation of heat loss availability as a function of crank angle for different speeds. It can be seen that the combustion process has the greatest impact on the heat loss availability. In the rest of the cycle, the value for heat transfer is small because of the small difference between the in-cylinder gas temperature and the wall temperature. During combustion, when the maximum temperature is reached, the heat transfer from the engine gases to the cylinder walls is high. By increasing the engine speed, heat loss availability decreases. When the engine speed increases, reduction in the duration of cycle evolution causes the reduction of heat transfer.

Figure 7 shows the variation of heat loss availability as a function of the engine speed. Similar result for DI diesel engine is gained by Abbasi *et al.* [12] that is illustrated in fig. 8.

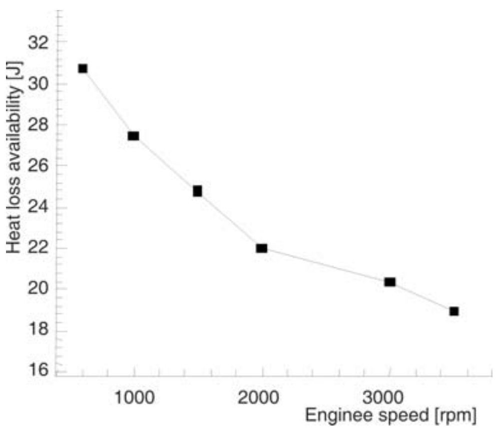

Figure 7. The effect of engine speed on heat loss availability

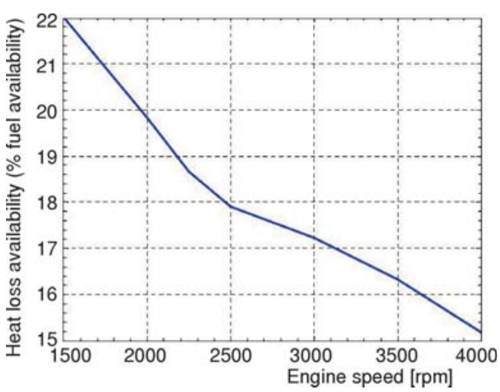

Figure 8.The effect of engine speed on heat loss availability [12]

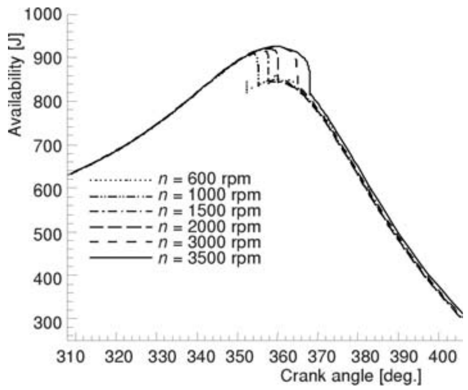

Figure 9. Total availability under various engine speeds

Figure 9 states that the increase in the engine speed causes an increase in total availability. It can be seen that total availability in the beginning of the cycle is more than its end because useful fuel energy releases during chemical reaction. In compression course, total availability is increased due to the work done by piston. In combustion duration that happens immediately, useful fuel energy which is hiding in chemical bonds, releases and transforms to thermal energy in an isochore process. This event causes the irreversibility of the process and as a result, total availability reduces. In expansion course, since the percentage of the availability is transformed to the expansion work, availability decreases. At the end of cycle, availability indicates available work from in-cylinder gases after the end of the cycle. If working fluid during the reversible process reaches the dead state, the so-called availability can be reached. Turbochargers transform only a part of this exergy to work, since they can decrease the outlet gas state only to the dead state pressure. In order to completely transform the outlet exergy to work, a turbocharger and then a lower cycle can be used to reach the outlet gas temperature to the dead state temperature.

If engine speed is low, by fixing the other parameters like inlet temperature, compression ratio, and equivalence ratio, ignition starts before TDC, so after the ignition, since engine is in the compression course, availability increases after ignition again, until it reaches TDC.

The relationship between entropy generation per cycle and engine speed is depicted in fig. 10. By increasing the engine speed, at first, the entropy generation increases and then by increasing the engine speed more, the entropy generation reduces. The highest level of entropy is generated at the speed around 2500 rpm. Similar result for DI diesel engine is gained by Abbasi *et al.* [12] that is illustrated in fig. 11. The entropy generated during combustion corresponds to the entropy increase due to the chemical reaction taking place inside the engine cylinder and

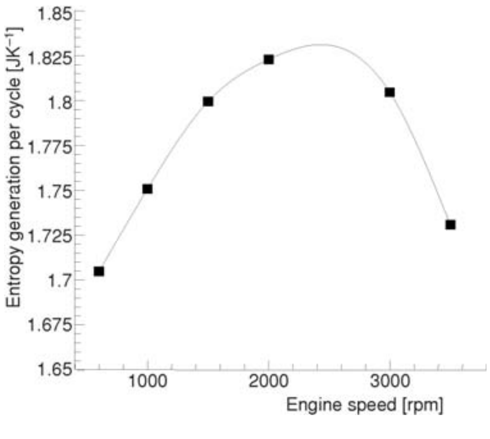

Figure 10. The effect of engine speed on entropy generation per cycle

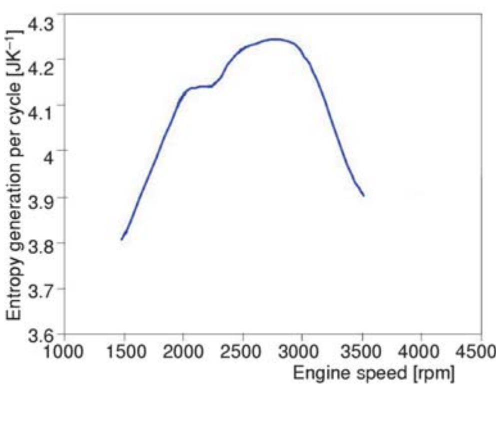

Figure 11. The effect of engine speed on entropy generation per cycle [12]

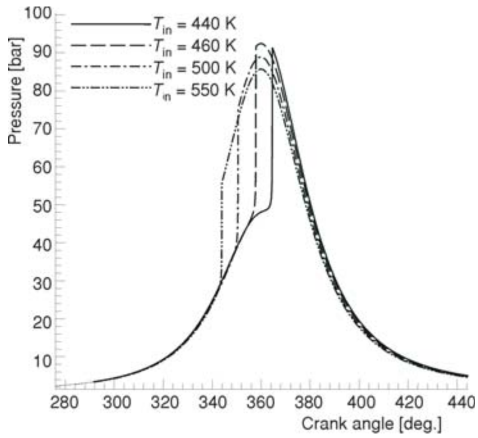

Figure 12. In-cylinder pressure under various inlet charge temperatures

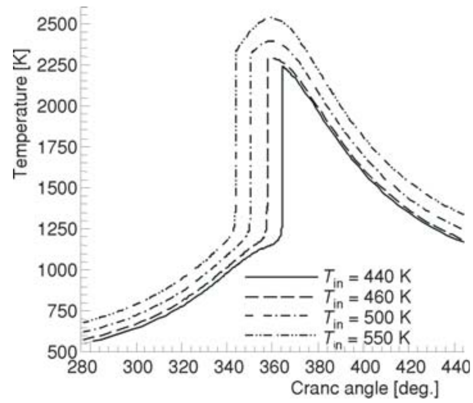

Figure 13. In-cylinder temperature under various inlet charge temperatures

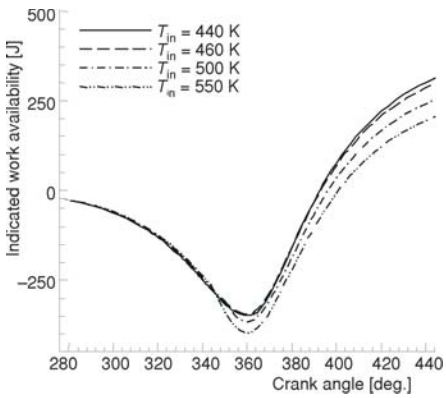

Figure 14. Indicated work availability under various inlet charge temperatures

heat transferred within that mass of gas. It depends mainly on three variables: the amount of burned fuel, the temperature, and the pressure of the gases inside the engine.

Ignition timing in HCCI engines is dominated by thermo-kinetic reactions that are dependant on the charge properties such as inlet charge temperature. In this part, the engine speed will be fixed at 1500 rpm and the inlet charge temperature varies from 440 K to 550 K and its effects on the energy and exergy terms will be investigated.

Figure 12 shows the variation of in-cylinder pressure as a function of crank angle under various inlet charge temperature. Two different states can be seen in this figure. One in the low inlet charge temperature, that inlet charge temperature increase causes an increase in the maximum in-cylinder pressure and auto-ignition takes place close to or after top dead center. In the other case, which the ignition starts before top dead center, as inlet charge temperature increases, maximum in-cylinder pressure reduces.

In fig. 13 it is indicated that an increase in the inlet charge temperature increases the in-cylinder temperature. An increase in the inlet charge temperature reduces trapped mass and volumetric efficiency, which in turns adversely affects torque and power output. Advanced ignition, which increases compression effort, combined with reduced volumetric efficiencies leads to a reduction in net indicated thermal efficiency. The best combustion timing and likely varies depending on the operating condition.

Figure 14 states that an increase in the inlet charge temperature leads to a decrease in the indicated work availability. Increase of the inlet charge temperature indeed decreases the pressure level during the combustion, which leads to reduction of the indicated work availability.

Figure 15 shows that an increase in the inlet charge temperature leads to an increase in the heat loss availability. Increase of the inlet charge temperature causes the gas temperature level to be raised and thus the combustion process will happen at the higher temperature, which leads to an increase in the heat loss availability.

Figure 16 reveals that an increase in the inlet charge temperature, leads to an increase in the total availability. The highest amount of exergy can be seen at the TDC. According to the figure, as the inlet charge temperature increases, the exergy has two picks. The first one shows the mixed auto-ignition and indicates the exergy generated by combustion. The second pick happens at the TDC which is a result of more increase in the pressure from auto-ignition to the end of expansion course. When the exergy analysis is concerned, inlet charge temperature increase is desirable and causes an improvement the engine operation. While as the temperature exceeds a known level and as discussed earlier, maximum pressure and indicated work availability decreases. So when the energy analysis is concerned, inlet charge tempe- rature increase is undesirable.

Figure 17 states that an increase in the inlet charge temperature leads to a decrease in the entropy generation per cycle. This result can be explained by referring to eq. (13). When an increase is applied in the inlet charge temperature the increase in the entropy of the inlet and outlet gas (S_{in} and S_{out}) are almost equal. (Indeed the difference of the increase of the inlet and outlet gas entropy can be ignored when the inlet charge temperature is raised). But the decrease in the total irreversibilities which is issue of the increase in the inlet charge temperature, is more than the increase in the heat loss availability. Hence, an increase in the inlet charge temperature leads to a decrease in the amount of the entropy generation per cycle. Similar result for DI diesel engine is gained by Abbasi *et al*. [12].

Conclusions

In this work, the influences of the inlet charge temperature and the engine speed are studied on the first and second laws of thermodynamics in an HCCI engine. For this purpose, a single zone thermo-kinetic model was used and tested favorably against experimental results. The results show that an increase in the inlet charge temperature causes the maximum pressure, indicated work availability and en-

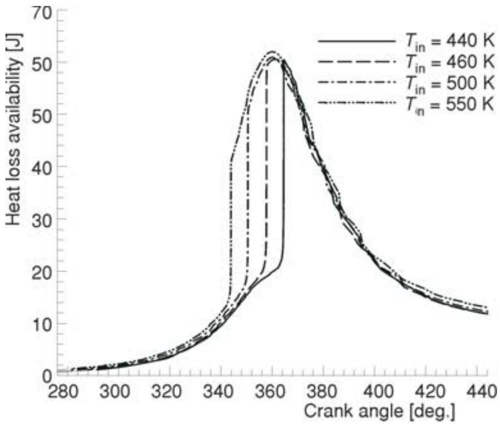

Figure 15. Heat loss availability under various inlet charge temperatures

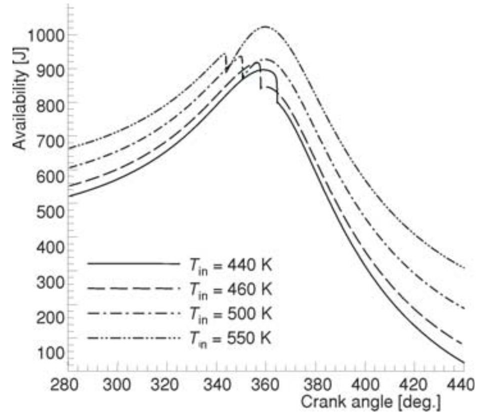

Figure 16. Total availability under various inlet charge temperatures

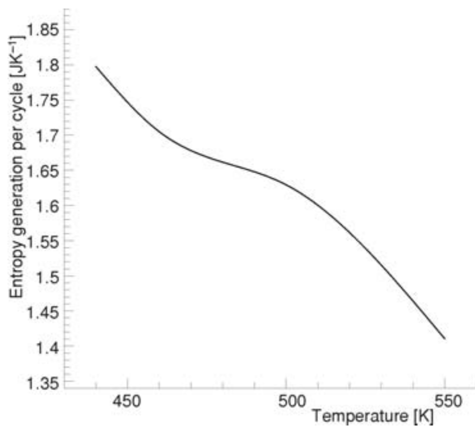

Figure 17. The effect of inlet charge temperature on entropy generation per cycle

tropy generation per cycle be reduced and the in-cylinder temperature, heat loss availability and total availability be increased. Also the results show that an increase in the engine speed causes the availability be increased and the heat loss availability be decreased. When the engine speed increases, reduction in the duration of cycle evolution causes the reduction of heat transfer.

According to the above results, by finding an optimum inlet charge temperature, it is possible to achieve a good balance between the first and second law terms, which leads to the better engine design.

Nomenclature

A – availability/exergy, [J]
A_s – in-cylinder surface area [m^2]
a_{fch} – specific availability/exergy, [Jkg^{-1}]
C_1 – constant value, [–]
C_2 – constant value, [–]
$C_{p,i}$ – specific heat capacity of the ith specie, [kJkg^{-1}K^{-1}]
h_c – convective heat transfer coefficient, [Wm^{-2}K^{-1}]
h_i – enthalpy of the i^{th} specie, [kJkg^{-1}]
I_{total} – total irreversibility, [J]
L – instantaneous cylinder height, [m]
N – number of moles, [mol]
P – pressure, [bar]
P_{cyl} – in-cylinder pressure, [bar]
P_{mot} – motoring pressure, [bar]
P_r – initial pressure, [bar]
Q – heat transfer, [J]
R_u – universal gas constant, [kJkg^{-1}K^{-1}]
S_{gen} – entropy generation, [JK^{-1}]
S_p – piston speed, [ms^{-1}]
s – specific entropy, [Jkg^{-1}K^{-1}]
T_{cyl} – in-cylinder temperature, [K]
T_g – gas temperature, [K]
T_r – initial temperature, [K]
t – time, [s]
U – internal energy, [J]
V_d – displacement volume, [m^3]
V_r – initial volume, [m^3]

Greek symbol

$\alpha_{scaling}$ – scaling factor, [–]
ϕ – crank angle, [deg.]
ω – local gas velocity, [ms^{-1}]

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