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Availability analysis of n-heptane and natural gas blends combustion in HCCI engines

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ABSTRACT

One of the major problems associated with HCCI combustion engine application is lack of direct control for combustion timing. A proposed solution for combustion timing control is using a binary fuel blend in which two fuels with different auto-ignition characteristics are blended at various ratios on a cycle-by-cycle basis.

The aim of this research is to investigate the exergy analysis of HCCI combustion when a blended fuel, which consists of n-heptane and natural gas, is used. In order to accomplish this task, a single-zone combustion model has been developed, which performs combustion computations using a complete chemical kinetics mechanism.

The study was carried out with different percentages of natural gas in blended fuels and EGR (exhaust gas recirculation) ranging from about 45 to 85 percent and 0 to 40 percent, respectively. The results reveal that, when mass percentage of natural gas increases, exergy destruction is decreased increasing the second-law efficiency. Introducing EGR into the intake charge of dual fuel HCCI engine up to some stage (optimum value) enhances the second-law performance of the engine in spite of a reduction in work.

1. Introduction

HCCI (Homogenous Charge Compression Ignition) combustion is a well-defined and well-understood technique with applications for the future of internal combustion engines both in mobile and stationary applications. HCCI combustion was first introduced by Onishi et al. [1] in a 2-stroke engine under the name of ATAC (Active-Thermo Atmosphere Combustion). Najt and Foster [2] in 1983 operated a 4-stroke HCCI combustion engine.

HCCI combustion is the auto-ignition of a highly diluted (with excess air and/or exhaust gas recirculation, EGR) air/fuel mixture at elevated intake temperature and/or compression ratio. Compared to spark ignition combustion engine, the fuel conversion efficiency is higher as the mixture is highly diluted, compression ratio is higher and the throttling losses are reduced [3–5]. In this type of combustion, both nitrogen oxides and soot emissions are reduced to near zero due to the formation of homogeneous lean mixture and the presence of large amount of EGR in the cylinder [6].

As HCCI combustion is governed by chemical kinetics [7], there is no direct way to control HCCI combustion timing. Combustion timing control is required for an optimized HCCI combustion. The optimized HCCI combustion engine can produce better combustion, performance and emission characteristics. HCCI combustion timing is a function of the engine intake initial conditions, compression ratio and fuel auto-ignition chemistry [7]. The latter can be controlled by blending fuels with different auto-ignition characteristics, so that various combustion timings can be obtained on a cycle-by-cycle basis by altering the blend ratio.

Several combinations of fuels including hydrocarbons, alcohols and reformer gas were used by researchers to control HCCI combustion timing [8-11]. For example, Hosseini and Checkel [12] studied dual fuel HCCI combustion engines using some blends of reformer gas (hydrogen and carbon monoxide mixture) with a range of fuels with various auto-ignition tendency including natural gas, n-heptane, and iso-octane. It was found that the reformer gas can be used to control HCCI combustion timing when it is blended with low octane number fuels which have strong low temperature heat release auto-ignition behavior.

In order to analyze engine performance and pollutant emission parameters, the first-law of thermodynamics is mostly used. This law does not consider the quality of energy content of a system. During the last 20 years, it has been understood that traditional first-law theory, often fails to give a good insight into the engine's

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Nomenclature

$\overline{a}$	molar specific chemical availability (J/mol)
a	mass specific chemical availability (J/kg)
A	availability (J)
a_h	heat transfer constant
b_h	heat transfer constant
c	heat transfer constant
C_v	specific heat at constant volume (J/kg K)
D	cylinder bore (m)
MW	molecular weight (kg/kmol)
$\overline{g}$	molar specific Gibbs function (J/mol)
G	Gibbs function (J)
$\overline{h}$	molar specific enthalpy (J/mol)
I	availability destruction (J)
V_c	clearance volume (m^3)
K	thermal conductivity of gas (W/mK)
m	mass (kg)
R	ratio of the connecting rod length to the crank radius
r_c	compression ratio
N	number of mole (mol)
P	pressure (N/m^2)
$P^{(r)}$	partial pressure (N/m^2)
Q	heat loss (J)
$\dot{q}$	heat flux (W/m^2)
$\overline{R}$	universal gas constant (kJ/kmol K)
Re	Reynolds number
$\overline{s}$	molar specific entropy (J/mol K)
S	entropy (J/K)
t	time (s)
T	temperature (K)
U	internal energy (J)
V	volume (m^3)
y	mole fraction of species
$\dot{\omega}$	molar rate of species (mol/m^3.sec)
E	exergy (J)
η_{II}	second-law efficiency
k	any species
n	total number of species in the mixture

Greek

θ	crank angle (deg)
φ	Total equivalence ratio
μ	chemical potential (J/mol)

Subscripts

0	dead state, or environment state
w	wall
Ch	chemical
Diff	diffusion
Red	reduction
TM	thermomechanical
Ox	oxidation

Superscripts

0	restricted dead state

Abbreviations

CA	degrees crank angle
BTDC	before top dead center
EVO	exhaust valve opening
W	associated with work transfer
IVC	inlet valve closing
LHV	lower heating value
rpm	revolutions per minute
EGR	exhaust gas recirculation
EPC	exergy performance coefficient

operation [13]. Therefore, the second-law analysis should be coupled to the first-law one. Availability is the amount of the energy in a system that is available for useful work [14]. Unlike energy, availability can be destroyed in processes such as combustion. In a dual-fuel HCCI engine, irreversibilities can occur due to various irreversible phenomena, such as combustion of natural gas (NG) and n-heptane fuels, heat transfer through a finite temperature difference, mixing, throttling, friction, and etc. An engine can lead to a more efficient operation through reduced irreversibility sources in it [15].

Over the years, reports on the detailed use of the second-law of thermodynamics in internal combustion engines have been published [16-19]. Conclusions of most of these studies have been collected and presented in detail in a recent review paper [20].

Caton [15] used an adiabatic, constant volume system to analyze availability during combustion process. It was shown that, the destroyed availability due to the combustion process ranged between about 5 and 25 percent of the original reactant availability. Also, the effects of changes in temperature, pressure and equivalence ratio during the combustion process on the terms of availability were examined.

Van Gerpan and Shapiro [21] presented a second-law analysis of the combustion process in a diesel engine using a single-zone model. They carried out a parametric study to reveal the effects of combustion timing, mass burning rate, and heat transfer rate on the availability destruction. In their study, the chemical availability was shown to be significant and necessary to obtain an accurate estimate of irreversibility.

Rakopoulos and Kyritsis [22] used a method developed for both combustion irreversibility and working medium availability computations in a high speed, naturally aspirated, four stroke internal combustion engine cylinder. Results of this study showed that the superseding fuels such as methane and methanol have better competence as compared with dodecane fuel.

Using a zero-dimensional model, Rakopoulos and Kyritsis studied computationally the exergy balance during combustion of hydrogen-enriched natural and landfill gases as fuels in combustion engine cylinder [23]. This work showed that, from the second-law point of view, hydrogen combustion was qualitatively different than the combustion of hydrocarbon fuels. Results of this study revealed a monotonic decrease in combustion irreversibilities by increasing hydrogen component of CH_4–H_2 mixture in an engine chamber.

Hosseinzadeh et al. [24] used a quasi-two-zone combustion model, combined with the detailed chemical kinetics scheme, to study the second-law analysis of a dual-fuel engine supplied with natural gas and diesel fuels at part load condition. Then different cases of EGR are applied to the availability terms. The results indicated that, Radical, thermal and combined cases of EGR have positive effects on availability terms. With employment of these cases of EGR, the combustion process improves due to enhancement of the oxidation process in lean mixtures.

From the previous brief survey, it can be concluded that the defined reactions among the related species in the combustion models were in equilibrium. In general, the chemical equilibrium assumption is not valid for the formation of pollutants [22]. In

recent years, chemical kinetic modeling has become an important and powerful tool to analyze combustion processes. Such computer models have contributed to a better understanding and solution of long standing practical combustion problems in HCCI engines [25,26].

Notwithstanding the numerous amount of work in the 1st law analysis of combustion in HCCI engines, there is a lack of information on the availability analysis of these engines. The present work aims to dress this lack of information by performing an availability analysis for compression, combustion and expansion processes in a dual-fuel HCCI engine. The fuel considered in the engine was a blend of n-heptane and natural gas fuels at various ratios ranging from 0 to 100 percent. Utilizing combined chemical kinetics mechanism and laws of thermodynamics, a single-zone combustion model is developed and used in this investigation. More attention was paid to the effect of EGR on availability balance of the engine in particular to define the optimum EGR amount for the considered case in this study.

2. Governing equations of single-zone combustion model

2.1. First-law (energy) analysis

The modeling was performed for the closed part of the HCCI engine cycle where in-cylinder mass remains constant. Therefore:

$$\frac{dm}{dt} = \sum_{k=1}^{n} \dot{m}_k = 0 \tag{1}$$

Net production rate of each of species is also as include:

$$\frac{dm_k}{dt} = \dot{\omega}_k MW_k V \tag{2}$$

The cylinder pressure is calculated at each CA step using the ideal gas state equation:

$$PV = \frac{m}{MW}\bar{R}T \tag{3}$$

Cylinder volume change equation relative to time is as follows:

$$\frac{dV}{dt} = V_C\left[\frac{1}{2}(r_C - 1)\left(\sin\theta\frac{d\theta}{dt} - \frac{1}{2}\left(R^2 - \sin^2\theta\right)^{-\frac{1}{2}}(-\sin 2\theta)\frac{d\theta}{dt}\right)\right] \tag{4}$$

Energy conservation equation is given as:

$$mc_V\frac{dT}{dt} + \sum_{k=1}^{n}\dot{m}_k u_k = -P\frac{dV}{dt} + \frac{dQ}{dt} \tag{5}$$

Heat flux through the combustion chamber boundary, the Annand's correlation [27] is:

$$\dot{q} = \frac{a_h K}{D}\mathrm{Re}^{b_h}(T - T_w) + c_h\left(T^4 - T_w^4\right) \tag{6}$$

Where T is the cylinder mixture temperature, T_w the wall temperature and a_h, b_h and c_h are the user defined constants. Based on our study, the constant a_h was estimated to be 0.685. This value was obtained by validating the simulation results from single zone combustion model (SZCM) with the experimental ones.

The chemical kinetic model previously reported by the authors [28] for n-heptane and natural gas blends was used in this paper. The model is consisted of 464 chemical reaction steps and the following 76 chemical species:

(1)C_7H_{16}, (2)CO, (3)H, (4)H_2, (5)CH_4, (6)CH_3, (7)CH_3O, (8)CH_2CO, (9)CH_2, (10)CH_2O, (11)CH_3O_2, (12)CH_4O_2, (13)HCO, (14)HCCO, (15)C_7H_{15-1}, (16)C_7H_{15-2}, (17)$C_7H_{15}O_2$, (18)$C_7H_{14}O_2H$, (19)$C_7H_{14}O_2HO_2$, (20)C_7KET_{21}, (21)C_6H_{12}, (22)$C_5H_{11}CHO$, (23)$C_5H_{11}CO$, (24)C_5H_{11}, (25)C_4H_9, (26)C_4H, (27)C_4H_2, (28)C_4H_3, (29)C_3H_7, (30)C_3H_6, (31)C_3H_5, (32)C_3H_4, (33)C_3H_3, (34)C_3H_2, (35)C_2H, (36)C_2H_2, (37)C_2H_3, (38)C_2H_4, (39)C_2H_5, (40)C_2H_6, (41)C_3H_8, (42)CH_2CHO, (43)CH_3CHO, (44)CH_3CO, (45)CH_2OH, (46)C, (47)CH, (48)HCCOH, (49)CH_3OH, (50)$CH_2(S)$, (51)NH, (52)NH_2, (53)NH_3, (54)NNH, (55)CN, (56)HCN, (57)H_2CN, (58)HCNN, (59)HCNO, (60)HOCN, (61)HNCO, (62)NCO, (63)O, (64)OH, (65)HO_2, (66)H_2O_2, (67)N_2O, (68)NO, (69)N, (70)NO_2, (71)HNO, (72)O_2, (73)N_2, (74)CO_2, (75)H_2O, (76)AR

2.2. Second-law (exergy) analysis

The availability of a system is defined as the maximum amount of work obtainable when a system is brought to thermal, mechanical and chemical equilibrium with its environment by means of reversible processes while exchanging heat with only environment. The availability of a system is divided into two parts: the thermomechanical availability and the chemical availability [14,20].

2.2.1. Gibbs function

This thermodynamic property represents the chemical potential of the substance in a given state and becomes very useful in the calculation of available work in a chemical reaction process. For an ideal gas mixture, the molar specific Gibbs function, evaluated at mixture temperature and partial pressure of species in the mixture is defined as [14,20]:

$$\begin{aligned}\mu_k &= \bar{g}_k\left(T, P_k^{(r)}\right) = \bar{g}_k(T, y_k P) = \bar{h}_k(T) - T\bar{s}_k(T, y_k P)\\ &= \bar{h}_k(T) - T\left[\bar{s}_k^0(T) - \bar{R}\ln\left(\frac{y_k P}{P_0}\right)\right](k = 1, \ldots, n)\end{aligned} \tag{7}$$

2.2.2. Definitions of availability terms

In general the total availability of a closed system is defined as [20]:

$$A = U + P_0V - T_0S - G_0 = U + P_0V - T_0S - \sum_{k=1}^{n} N_k\mu_{k,0} \tag{8}$$

In these expressions, kinetics and potential energies have been neglected.

2.2.3. Thermomechanical availability

Following usual conventions [14,20], thermomechanical availability of a system is defined as:

$$\begin{aligned}A_{TM} &= (U - U^0) + P_0(V - V^0) - T_0(S - S^0) = U + P_0V - T_0S - G^0\\ &= U + P_0V - T_0S - \sum_{k=1}^{n} N_k\mu_k^0\end{aligned} \tag{9}$$

2.2.4. Chemical availability

In general, chemical availability can be calculated from the following equation [20]:

$$A_{Ch} = A - A_{TM} = G^0 - G_0 = \sum_{k=1}^{n} N_k\left(\mu_k^0 - \mu_{k,0}\right) \quad (10)$$

Chemical availability can be divided into oxidation availability, reduction availability and diffusion availability [20]. Therefore, the total chemical availability is:

$$A_{Ch} = A_{Ox} + A_{Diff} + A_{Red} \quad (11)$$

The three parts of chemical availability is expressed separately as follows:

2.2.4.1. Oxidation availability. The species number 1–62 can be burned and converted into environmental species. The general reaction equation is:

$$C_aH_bO_cN_d + \left(a + \frac{b}{4} - \frac{c}{2}\right)O_2 \rightarrow (a)CO_2 + \left(\frac{b}{2}\right)H_2O + \left(\frac{d}{2}\right)N_2 \quad (12)$$

Using the above reaction, molar chemical availability of the unburned species can be defined as [14,20]:

$$\begin{aligned}\overline{a}_{Ox} = {} & \overline{g}_{C_aH_bO_cN_d}(T_0,P_0) + \left(a + \frac{b}{4} - \frac{c}{2}\right)\overline{g}_{O_2} - (a)\overline{g}_{CO_2}(T_0,P_0) \\ & - \left(\frac{b}{2}\right)\overline{g}_{H_2O}(T_0,P_0) - \left(\frac{d}{2}\right)\overline{g}_{N_2}(T_0,P_0) \\ & + \overline{R}T_0 \ln\left[\frac{\left(y_{O_2}^0\right)^{a+\frac{b}{4}-\frac{c}{2}}}{\left(y_{CO_2}^0\right)^{a}\left(y_{H_2O}^0\right)^{\frac{b}{2}}\left(y_{N_2}^0\right)^{\frac{d}{2}}}\right] + \overline{R}T_0 \ln y_k \end{aligned} \quad (13)$$

Therefore, total oxidation availability is defined as [20]:

$$A_{Ox} = \sum_k N_k \overline{a}_{Ox,k} (k = 1, \ldots, 62) \quad (14)$$

2.2.4.2. The reduction availability. The reduction term concerns with the species number 63–71 such as OH, NO, N and etc. which can be reduced to environmental species. To calculate the reduction exergy of these species, the general equation for chemical availability can be used as [20]:

$$A_{Red} = \sum_k N_k\left(\mu_k^0 - \mu_{k,0}\right) \quad (k = 63, \ldots, 71) \quad (15)$$

For example, the specie NO can be reduced to environmental species by following reaction:

$$NO \rightarrow \frac{1}{2}N_2 + \frac{1}{2}O_2 \quad (16)$$

Using the above reaction, the corresponding chemical potential at dead state can be calculated as follows:

$$\mu_{0,NO} = \frac{1}{2}\mu_{0,N_2} + \frac{1}{2}\mu_{0,O_2} \quad (17)$$

2.2.4.3. Diffusion availability. Diffusion availability of a system, as previously mentioned, concerns only with those species of system which are present in the environment. These species are assumed to be O_2, CO_2, H_2O, N_2 and AR. To calculate this availability, temperature, pressure and the composition of the environment (dead state) must be specified. In the present study, the temperature and pressure conditions of dead state are $T_0 = 298$ K and $P_0 = 1.0$ bar and the molar composition of the environment is: 20.35% O_2, 75.67% N_2, 3.03% H_2O, 0.3% CO_2 and 0.92% various other substances such as Argon.

Therefore, from Eq. (11) and the calculated molar specific Gibbs function at the restricted dead state and dead state, diffusion availability can be obtained as follows [20]:

$$A_{Diff} = \overline{R}T_0 \sum_k N_k \ln\left(\frac{y_k^0}{y_{k,0}}\right) (k = 72, 73, 74, 75, 76) \quad (18)$$

2.2.5. Engine cylinder availability balance

The availability balance equation applied for the closed system inside the cylinder, on crank angle basis, is expressed as follows [20,21]:

$$\frac{dA}{d\theta} = \frac{dA_W}{d\theta} - \frac{dA_Q}{d\theta} - \frac{dI}{d\theta} \quad (19)$$

Where, A_w is availability associated with work done by the system and it can be defined:

$$\frac{dA_W}{d\theta} = (p - p_0)\frac{dV}{d\theta} \quad (20)$$

This equation represents the rate of work availability that is equal to the rate of useful work done by the system.

Also, A_Q is availability associated with heat transfer across the system boundary. Its variation with crank angle is:

$$\frac{dA_Q}{d\theta} = \left(1 - \frac{T_0}{T}\right)\frac{dQ}{d\theta} \quad (21)$$

where T is in-cylinder gas mixture temperature.

3. Experimental set-up and engine specifications

The engine was a Waukesha CFR (Co-operative fuel research) single-cylinder engine. Details on engine specifications are shown in Table 1. The intake pressure was adjusted depending on the operating conditions. The throttle valve was kept wide open. A heater was installed inside the intake manifold in order to control the intake mixture temperature when needed. Intake mixture consisted of air, natural gas, n-heptane, and exhaust gas recirculation (EGR). Fuels were delivered in the intake using two port fuel liquid and gaseous injectors. The composition of natural gas is indicated in Table 2. Intake mixture temperature was set at constant value and monitored just before the intake valve. EGR line was taken immediately after the exhaust port and returned to the intake manifold after the heater and before the fuel injectors. EGR was controlled by a manual butterfly valve. Two port fuel gaseous and liquid injectors were installed in the intake port before the intake valve. A Kistler 6043A water-cooled pressure transducer was used to acquire pressure signal on a 0.1 CAD resolution. Fig. 1 shows the details of experimental setup.

Table 1
CFR engine specifications.

Parameter	Specification	Parameter	Specification
Engine type	Single-cylinder	Connecting rod (cm)	24
Displacement (cc)	612	IVO (CA)	10
Throttle	Fully open	IVC (CA)	214
Bore (cm)	8.26	EVO (CA)	500
Stroke (cm)	11.4	EVC (CA)	735

Table 2
Natural gas properties.

Property	Value
Normalized CH_4 dry molar fraction	95.39%
Normalized C_2H_6 dry molar fraction	1.90%
Normalized N_2 dry molar fraction	1.93%
Normalized CO_2 dry molar fraction	0.78%
Molar mass [g/mol]	16.76
Density at STP [kg/m^3]	0.748
H/C ratio	3.92
LHV [kJ/kg]	44,818

4. Description of the computational procedure

The aforementioned model was written in FORTRAN programming language. The solver code calculates the unknown variables (mass of species and mixture temperature and pressure), for a user-defined time step. The calculation is based on ideal gas theory, specified heat transfer model developed combined chemical kinetic mechanism and thermodynamic property models for gas mixtures. In order to reduce the time of computation, the chemical reactivity is considered to be negligible where the temperature is less than 600 K.

User-defined time step was fixed at 0.1 CA for the compression, combustion and expansion processes. The flowchart of the code developed by the authors is given in Fig. 2. Wide range of operating conditions used in this investigation is presented in Table 3.

5. Results and discussions

5.1. Baseline results

Fig. 3 shows a comparison between the predicted in-cylinder pressure with the corresponding experimental data for different considered cases. According to the diagrams of this figure, it can be concluded that the results of single-zone combustion model have a good compatibility with experimental data. Heat release rate is also included in these diagrams which indicates that, two phase combustion approaches to the single phase combustion by increasing natural gas mass percentage in the introduced blended fuel mixture.

Fig. 4 indicates variations of different cumulative availability terms with the crank position for different considered cases. The availability terms are considered in five parts: chemical availability, thermomechanical availability, work availability, availability transfer through heat and irreversibility. It can be seen that, during the compression process, the chemical availability of the mixture remains constant because the chemical composition of the cylinder charge does not change. The work availability is transferred to the cylinder charge and consequently the thermomechanical availability and consequently the total exergy increases during compression process. However, the availability transfer due to heat transfer via the cylinder wall is comparatively low. Also, the availability destruction due to the irreversibilites is insignificant during the compression process. From the beginning of the first stage of combustion process, which consists of low temperature oxidation reactions, the n-heptane begins to burn decreasing slightly the chemical availability of the mixture. It follows that the thermomechanical availability increases slightly with rising pressure and temperature of the cylinder charge. These changes are in such a way that, the total availability of the cylinder charge decreases very slightly which can be due to overcoming of reduction of fuel chemical exergy in comparison with increasing of thermomechanical exergy. As the piston moves towards the top dead center and also because of the first stage of n-heptane combustion, the work availability transfer increases. The availability transfer due to heat transfer from the combustion chamber in this stage is however negligible. During this stage, slight destruction of availability occurs, which is due to the irreversible nature of n-heptane oxidation process. From the beginning of the second stage of combustion process, which consists of high temperature oxidation reactions, the cylinder charge is immediately ignited. The chemical availability of the mixture decreases quickly due to the conversion of unburned species into combustion products. Work availability transfer may increase or decrease depending on the position of the piston during the second stage of combustion. However, the thermomechanical availability of the cylinder charge increases rapidly with the sudden rise of in-cylinder charge pressure and temperature. After this stage, the thermomechanical availability decreases, because the availability is transferred out of the system due to both work and heat transfers from the system. Availability destruction associated with this stage of combustion process, which is basically due to the irreversible nature of fuels oxidation process [22], is significant. In the expansion process, the change in chemical availability is not considerable. However, there could be some combustion of as incomplete combustion products and consequently the changes in partial pressure of environmental species in the cylinder charge. As the cycle proceeds, the thermomechanical

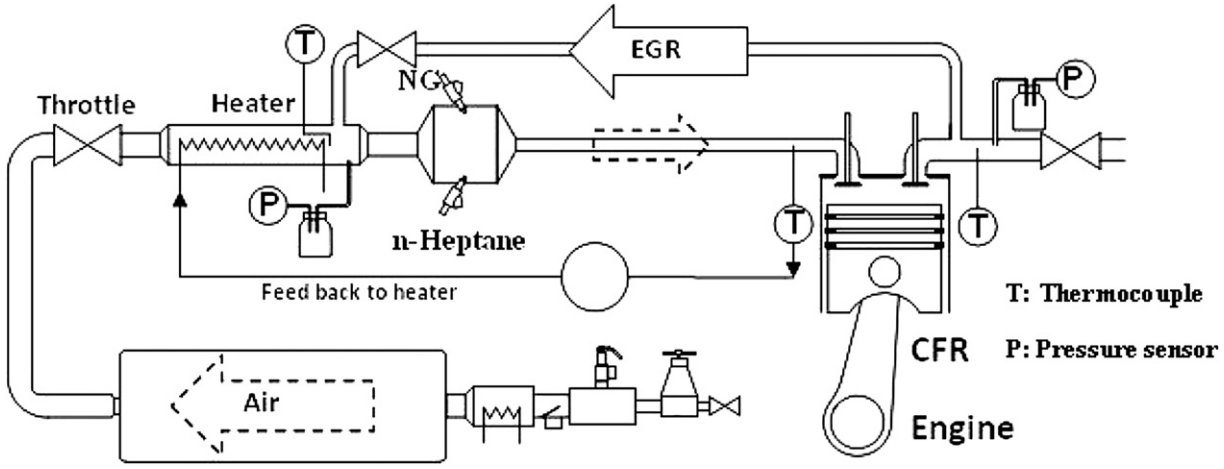

Fig. 1. Schematic of HCCI research facility at university of Alberta.

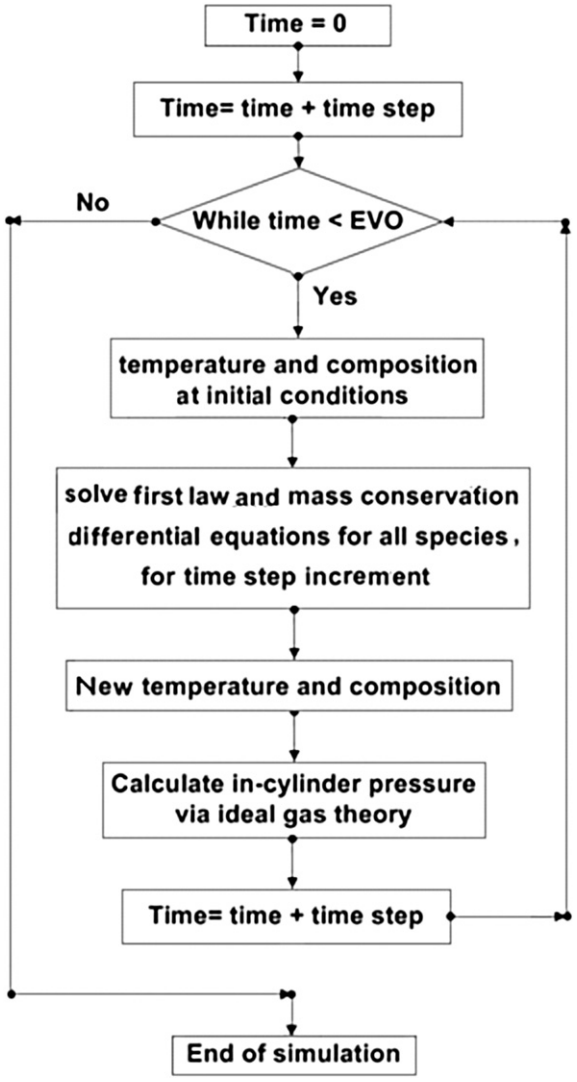

Fig. 2. Single-zone combustion model Flow chart.

availability decreases because of heat and work transfers from the system and the obtained values for the irreversibility associated with this process is relatively small.

Fig. 5, shows destructed exergy percent to the total inlet exergy introduced into the engine. This figure shows that by increasing mass percentage of natural gas, less exergy will be destructed by irreversible combustion process. This may be originated from reduction of the irreversible reactions which breaks up n-heptane to more simple hydrocarbons [22].

Table 3
CFR engine operating conditions for three considered cases.

	Case 1	Case 2	Case 3
NG mass fraction (%)	44.6	65.0	85.1
Equivalence ratio Φ	0.61	0.64	0.90
NG mass flow rate (mg/s)	32.5	36.91	62.25
n-heptane flow rate (mg/s)	40.4	19.86	10.91
% EGR	23.8	32.45	33.56
T_{IVC} (K)	393	413	413
P_{IVC} (bar)	0.97	1.05	0.94
Compression ratio	13.8	16	16
Engine speed (rpm)	800	800	800

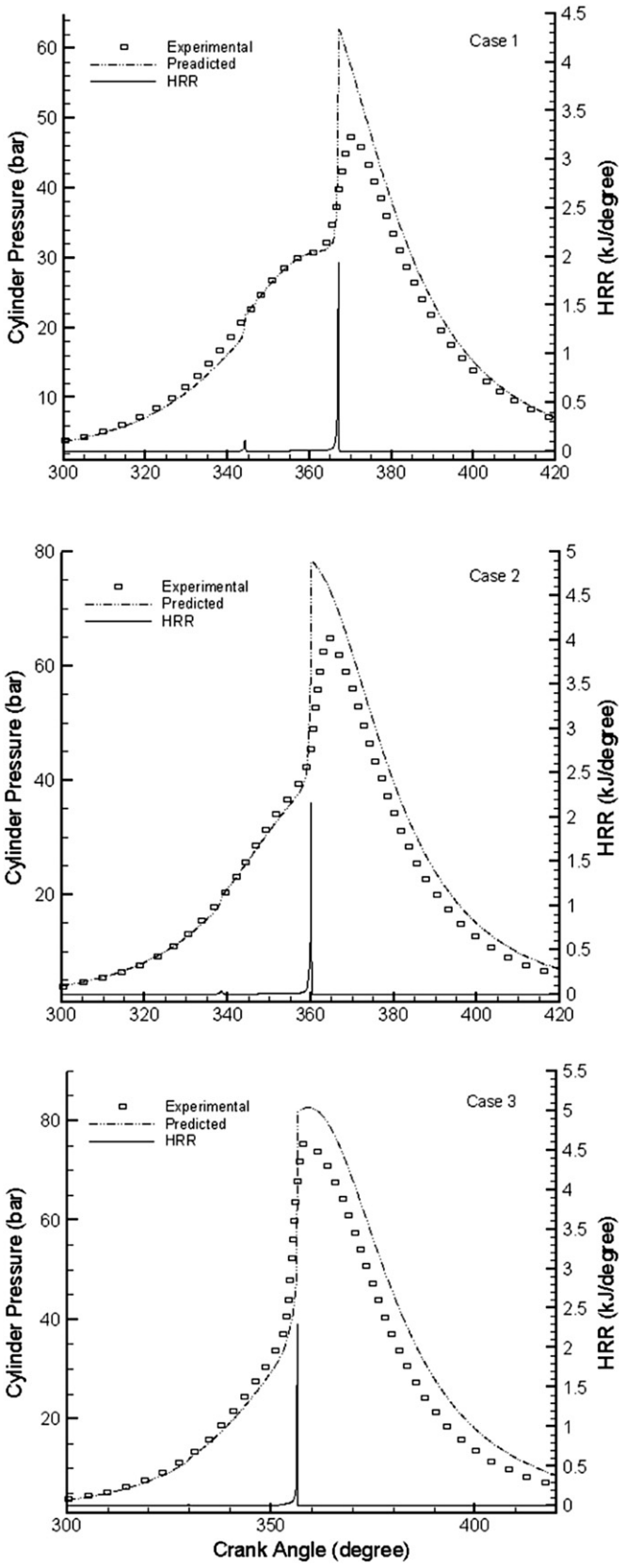

Fig. 3. Comparison of experimental and calculated pressure traces and heat release rate diagram for different considered cases.

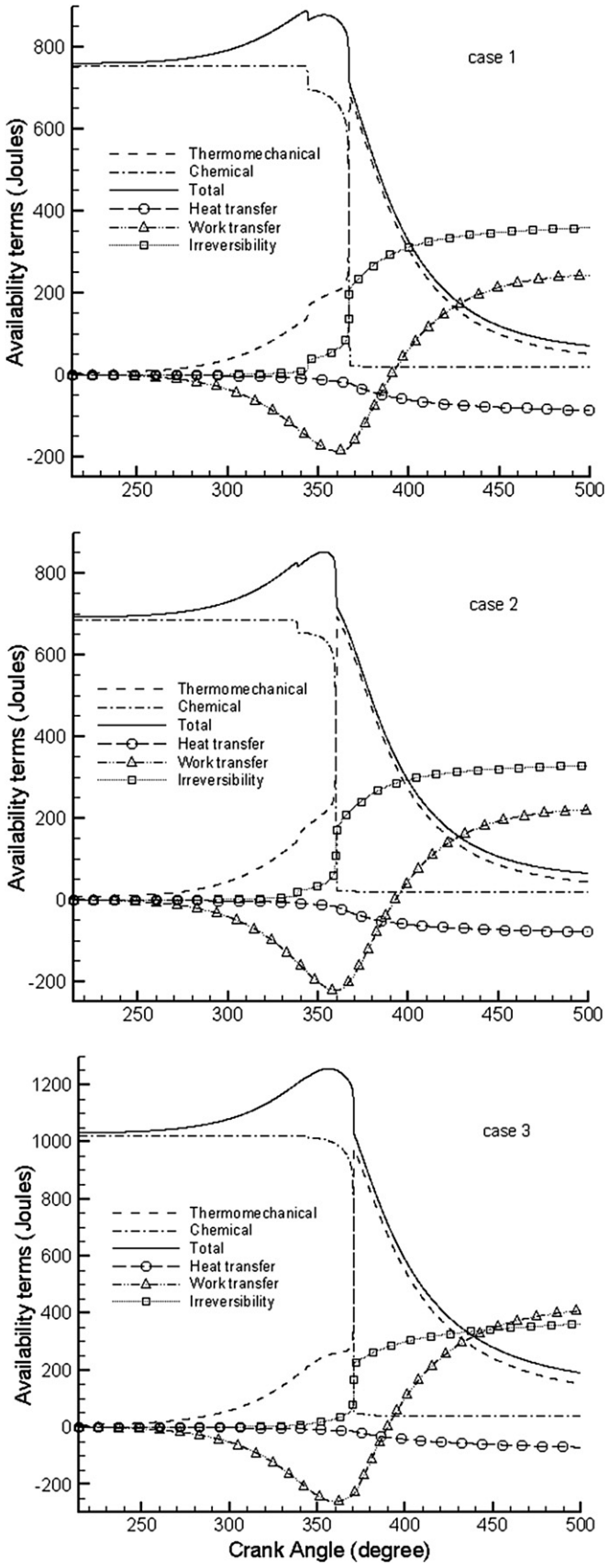

Fig. 4. Variations of cumulative availability terms for the cylinder charge with crank position for different considered cases.

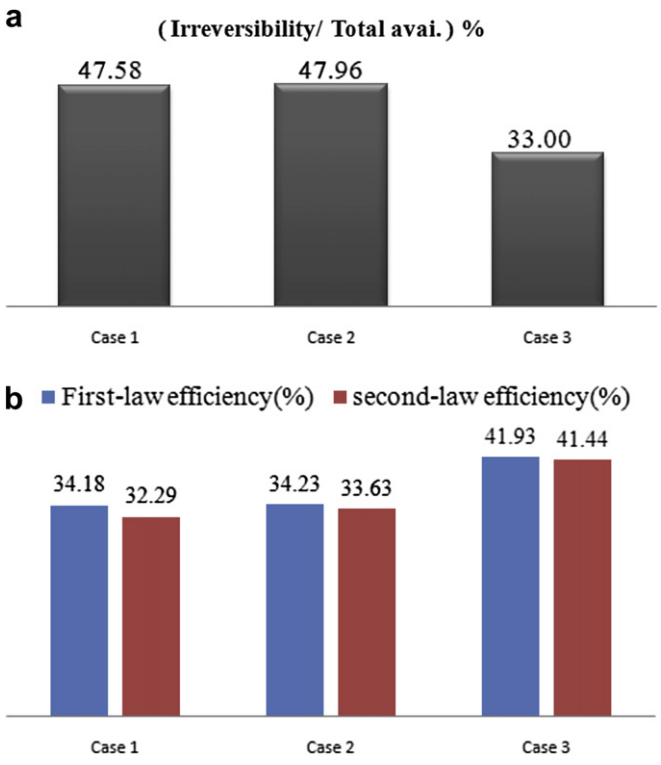

Fig. 5. Amounts of a) irreversibility relative to total inlet fuel availability and b) 1st and 2nd law efficiencies for the considered cases.

The second-law efficiency can be defined as the ratio of indicated work to the total input chemical availability. For the closed part of the cycle in a dual fuel HCCI engine, the second-law efficiency is defined as [14]:

$$\eta_{II} = \frac{W_{\text{indicated}}}{A_{\text{NG}} + A_{\text{n-heptane}}} \tag{22}$$

Case b of this figure shows the first and second-law efficiencies at various operating conditions. As it is evident from the figure, increasing mass percentage of natural gas will result in an increase

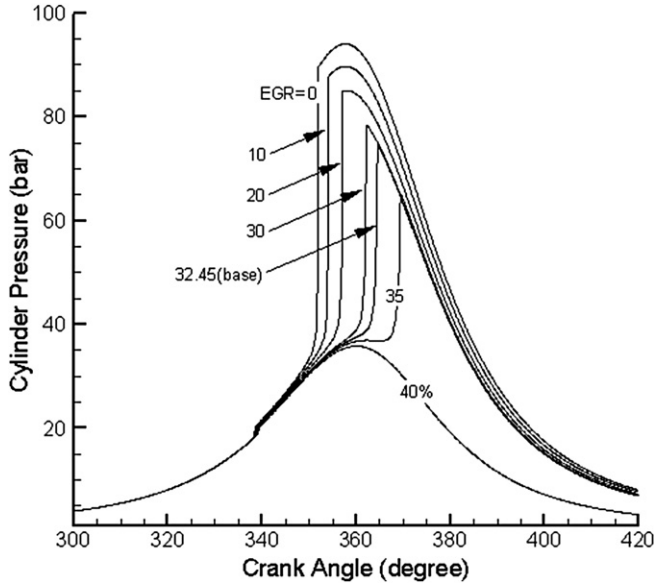

Fig. 6. Variations in the calculated cylinder pressure with crank position for different values of EGR.

of both first and second-law efficiencies which is due to the decrease in irreversibility.

5.2. Effect of EGR on availability terms

In this part of the paper, case number 2 is chosen as base case to investigate the effect of EGR on different availability terms. The percentage of EGR is altered from 0 to 40. Fig. 6 shows pressure variation versus crank angle for various values of EGR.

Fig. 7 shows the variations of different exergy terms against crank angle for various percentages of EGR. It can be seen from case a of this figure that, the thermomechanical exergy is decreased as EGR value increases. This is a consequence of EGR entry, which makes the in-cylinder mixture more diluted resulting in a lower temperature and pressure inside the cylinder.

The case b of Fig. 7 indicates the variations of chemical exergy versus crank angle as the EGR percentage changes. It is evident from this figure that, the chemical exergy of in-cylinder charge is reduced with increasing EGR percentage as less fuel enters the cylinder at higher EGR values.

The Case c of Fig. 7, shows work exergy variation with crank angle for various EGR percentages. The figure indicates that, the work exergy is decreased as EGR increases which is explained above.

The variation of in-cylinder charge exergy destruction (irreversibility) with crank angle at various EGR percentages is shown in case d of Fig. 7. The figure indicates that as EGR increases the exergy destruction is decreased which is due to the less amounts of introduced fuel available for combustion.

Fig. 8 indicates variations of 2nd law efficiency for different values of EGR. It can be concluded that this efficiency is increased by increasing EGR percentage as expected. However, the combustion process does not take place at EGR values above 40 percent. Therefore, exergetic efficiency reaches a zero value.

One of the important parameters in evaluating the performance of energy conversion systems is the ratio of useful exergy to

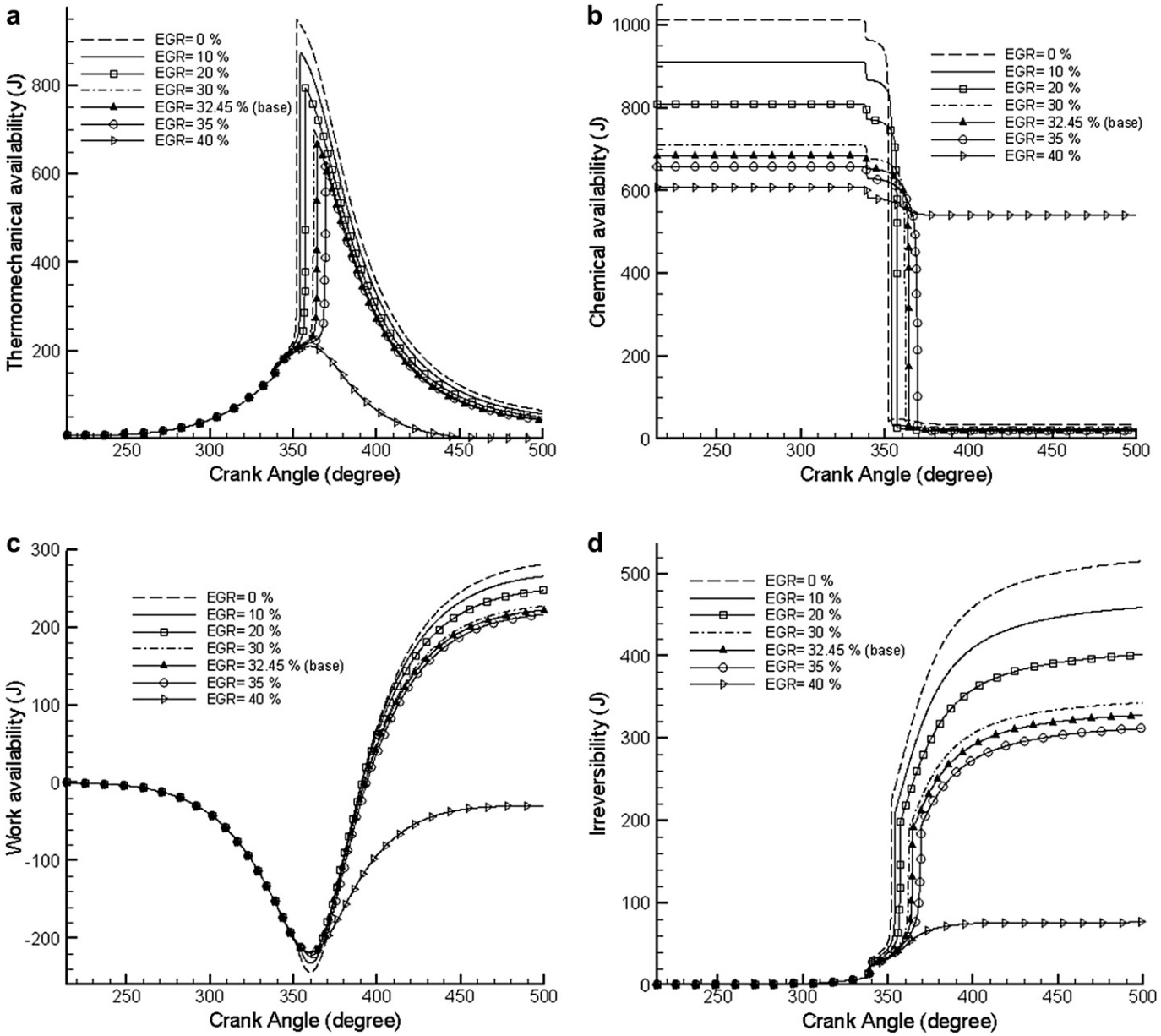

Fig. 7. Variations of the availability terms with crank position for different values of EGR.

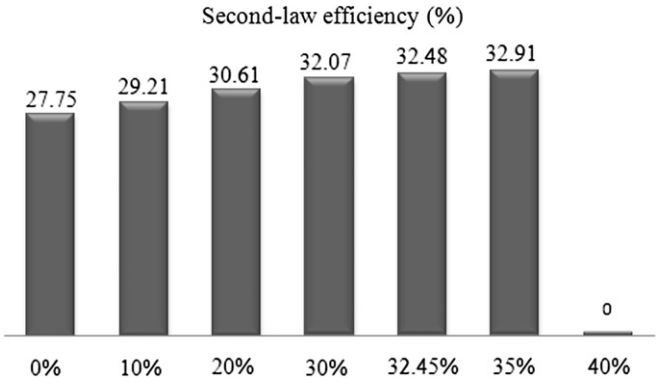

Fig. 8. Variations of the 2nd law efficiency versus EGR percentage for the considered case in dual fuel HCCI engine.

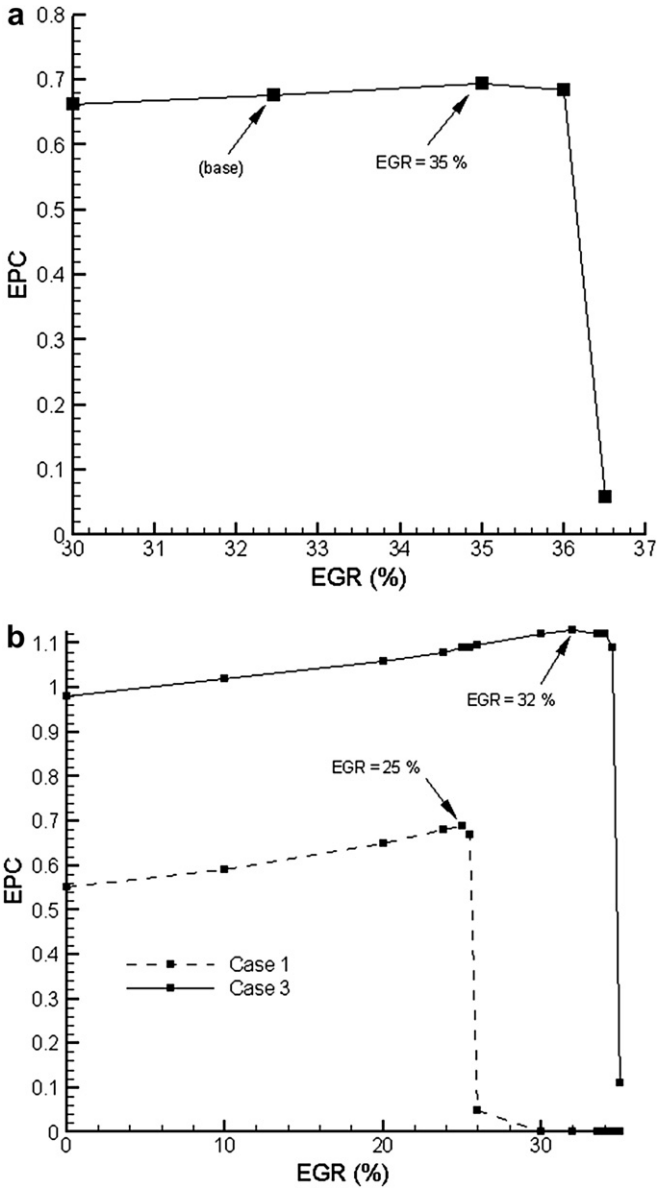

Fig. 9. Variation of the EPC versus EGR percentage for a) the considered case b) the other cases in dual fuel HCCI engine.

irreversibilities. This parameter is called EPC (exergetic performance coefficient) defined as [29]:

$$\mathrm{EPC} = \frac{W_{\mathrm{indicated}}}{E_{\mathrm{Destruction}}} \tag{23}$$

The EPC can be accounted as a powerful tool for defining the optimum amount of EGR that should be introduced into the cylinder charge to control HCCI dual fuel combustion. This is due to this fact that EPC considers both useful exergy and exergy destructions. The variations of EPC with percentage of EGR are shown in Fig. 9a indicating that an EGR value of 35 percent brings about the engine optimum performance for the considered case, from the view point of second-law of thermodynamics. Also, variations of EPC with percentage of EGR are shown in Fig. 9b for the other cases considered in this study which indicate the same trend as discussed above.

6. Conclusions

A single-zone combustion model, combined with the detailed chemical kinetics scheme, is developed for studying the second-law analysis of a HCCI engine supplied with different fractions of natural gas and n-heptane fuels. The study was carried out with different percentages of EGR ranging from 0 to 40 percent. The various availability components are calculated separately as a function of crank angle. The following conclusions are carried out to identify the best operating conditions of dual-fuel HCCI engine:

1- When mass percentage of natural gas in the fuel blend increases, exergy destruction is decreased increasing the second-law efficiency.
2- EGR could be one of the necessary techniques in controlling HCCI combustion. Therefore, the amount of introduced EGR can be defined by applying the availability analysis on the considered engine at different operating conditions.
3- Introducing EGR into the intake charge of dual fuel HCCI engine up to some stage (optimum value) enhances the second-law performance of the engine in spite of a reduction in work. The EGR values above this could deteriorate the engine performance.

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