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Thesis

Efficiency Analysis of Automotive Hydrogen Internal Combustion Engine Combined with a Steam Rankine Cycle

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Abstract

A hydrogen internal combustion engine (HICE) emits both heat and water from the combustion process. In this study, a new concept of heat recovery sub-system, which exploits the water exhausted from an automobile HICE as a working fluid for a steam power generation system based on the Rankine cycle has been introduced. In this cycle, the water separated from the HICE exhaust is evaporated and superheated by the exhaust waste heat of the HICE, and the water vapor is released to the atmosphere after it is used to produce power in a steam expander. The operating concept of the proposed recovery sub-system is described in this study, along with its potential power generated, and its beneficence to the overall thermal efficiency of the HICE. The recovery sub-system has been evaluated for various engine speeds using a fundamental thermodynamic model analysis. Two designs of the model have been examined; one with a condenser and another one without the condenser. The results showed that the design without a condenser is a cost-effective and simple approach, and its performance is comparable to another design. Both designs consumed almost equal amount of water as their working fluid. Consequently, it is concluded that the design without condenser is preferable for the recovery sub-system for HICE, which could enhance the overall thermal efficiency of the HICE from 27.2% to 33.6%, representing improvements of 2.9% to 3.7% from an HICE without any recovery sub-systems at engine speeds of 1500 to 4500 rpm.

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Nomenclature

Abbreviations

CVVT	continuous variable valve timing
FC	fuel cells
HICE	hydrogen fueled internal combustion engine
ICE	internal combustion engine
ORC	organic Rankine cycle
RS	recovery sub-system

Symbols

CO	carbon monoxide
$C0_2$	carbon dioxide
h	enthalpy (kJ/kg)
H_2	hydrogen molecule
H_2O	water molecule
m	mass flow rate (kg/s)
	nitrogen molecule
O_2	oxygen molecule
Q	heat (kW)
p	pressure (MPa)
$Qlhv$	low heating value of fuel (kJ/kg)
s	entropy (kJ/kg-K)
T	temperature (°C)
W	power (kW)

Greek Symbols

e	heat exchanger effectiveness
r	brake torque (Nm)
V	efficiency
A	air fuel ratio
n	mathematical constant, pi (value = 3.14159, or
co	angular velocity (revolutions per second, rps)

Subscripts

1	working fluid state at pump inlet, or inside water tank
2	working fluid state at pump outlet, or evaporator inlet
3	working fluid state at evaporator outlet, or expander inlet
4	working fluid state at expander outlet
5	working fluid state at condenser outlet
a	actual isentropic condition
BTE	brake thermal efficiency
C	condenser fan
co	cooling and other (losses)
E	expander
el	exhaust gas at evaporator inlet
^{eva}P	exhaust waste (passes through evaporator)
ew	exhaust waste (before reaching evaporator)
exh	exhaust waste (total from HICE)
/	fuel
G	generator
HX	heat exchanger
in	gained by working fluid (in evaporator)
liq	saturated liquid condition
overall	overall thermal for combined HICE and the recovery sub-system
P	pump
S	water separator
5	ideal (100%) isentropic condition
JW	separated water
required	additional water amount required
RS-I	recovery sub-system I
RS - II	recovery sub-system II
T	total amount of water (before separation process)
th	thermal
total	total amount of heat (from HICE combustion process)
^{va}P	saturated vapor condition
w	working fluid

Chapter 1

Introduction

1.1 Hydrogen as fuel

Hydrogen is known as the simplest and lightest of all chemical elements and the most spread in the universe. In nature, it exists only in combination with other elements, primarily with oxygen in water and with carbon, nitrogen and oxygen in living materials and fossil fuels. Through some kind of unbound processes, the molecular hydrogen can be produced by splitting those combined elements to respective molecules or atoms.

Currently more than 80% of the world energy supply comes from fossil fuels, resulting in strong ecological and environmental impacts. As fossil fuels are hydrocarbons, their combustion will produce $C0_2$, which has been considered as the most important contributor to radiative forcing in the atmosphere, resulting in a global warming or the so called greenhouse effect. Besides the use of fossil fuels lead to exhaustion of energy reserves and resources, now this is known as an important cause of air pollution and modification of the atmospheric composition, which then result to the climate changes and human health problems.

The Kyoto Protocol to the United Nations Framework Convention on Climate Change (UNFCCC) is amendments to the international treaty signed in 1992 on climate change, assigning mandatory emission limitations for the reduction of greenhouse gas emissions to the signatory nations, by either increase the energy conversion efficiency, or promote the alternatives to the carbon containing energy sources. In the other hand, hydrogen seems as an environmentally attractive fuel as it can be burned, or combined with oxygen in fuel cell without generating carbon dioxide ($C0_2$), and producing only water. In terms of function as an energy carrier, hydrogen seems similar to electricity which can provides useful energy with no environmental impact at the point of utilization, and will gain an importance in the near future.

Moreover, hydrogen is also viewed as a means to enhance energy security, as the global fossil fuels reserves are geographically concentrated, and there is increasing evidence that the peak in oil production will about to happen in the very near future [1, 2], Therefore, the use of hydrogen as an energy source creates diversifications of energy sources and the reduction of dependency on fossil fuels. Furthermore, through the introduction of this new energy source, it could improve the reliability of the energy supply and stabilize the energy market.

In this study, the utilization of hydrogen as an energy source is specifically emphasized for internal combustion engine (ICE) fuel used in automobile application. Table 1, summarizes the most important physical and combustion-related properties of hydrogen as compared to the other ICE's fuels (i.e., gasoline and methane). The original data and the other properties can be found in the source references [3, 4],

Table 1 - Hydrogen properties compared with methane and gasoline properties.

Property	Hydrogen	Methane	Gasoline
Density at 1 atm and 300K (kg/m^3)	0.082	0.717	5.11
Stoichiometric volume fraction in air (vol%)	29.53	9.48	1.65
Minimum ignition energy (mj)	0.02	0.28	0.25
Auto-ignition temperature (K)	858	813	-500-750
Adiabatic flame temperature (K)	2318	2190	-2470
Flammability limits in air (vol%)	4-75	5.3-15	1.2-6.0
Quenching distance (mm)	0.64	2.03	-2.0
Lower heating value (MJ/kg)	119.7	46.72	44.79
High heating value (MJ/kg)	141.7	52.68	48.29

As refer to the auto-ignition temperature of hydrogen, it seems to exceed the values for methane and gasoline. This means that the hydrogen particularly suited for spark ignition operation and unsuited for compression ignition. Therefore, the work of this study, hereafter deals exclusively with hydrogen spark-ignition internal combustion engine.

1.2 Hydrogen internal combustion engine

Currently, there are a number of available technologies associated with the use of hydrogen as an energy carrier. For automobile purposes, there are two potential technologies could be used, i.e., hydrogen fuelled internal combustion engines (HICE) and fuel cells (FC). The present work focuses on HICEs instead of FC for the following reasons:

- The internal combustion engine has benefited from a continuous development during more than a century and is still showing potential for further optimization. FC technology on the other hand is still in its infancy.
- This also reflects in the price, with a prohibitive cost for FC. Naturally, the conversion of an ICE to HICE increases its cost but this cost[1] is very low relative to a very new technology like FC. Using HICEs allows bi-fuel, or flex-fuel operation in which the engine can run on hydrogen as well as on gasoline and natural gases.
- FC are currently still handicapped by cold-start problems (freezing of the fuel cell stack) and the necessity of very pure hydrogen to avoid poisoning of the FC [5, 6]. The HICE however does not suffer from these problems. Although the most frequently acclaimed advantage of fuel cells is its high theoretical efficiency, the efficiency decreases as the load increases (the cell ohmic losses increase with the of the increase in cell's operational

[1] Additional cost is the modification cost of the HICE injection system and engine control unit, and possibly some changes to the ignition and crankcase ventilation system.

current density) [7]. This is not an important disadvantage for light-duty applications, but could become important for heavy duty.

- Furthermore, hydrogen fuelled ICEs also have the potential for an increased engine efficiency, with a demonstrated indicated efficiency of 52% for a hydrogen fuelled spark-ignition engine [8] and a power generation efficiency of 49% for a hydrogen fuelled compression-ignition engine [9].

In summary, the HICE and FC both have their own advantages and potential applications. In terms of existing capital investment and technology utilizations, the HICE is considered to be a primary power generation system that offers a feasible interim solution with more effectively than a FC system [8], and it can function as a transition technology to the fuel cells, or other better technologies.

There are two important aspects regarding the HICE: it produces a large amount of water[2] during its combustion process and the combustion temperature for hydrogen is higher than for gasoline [10]. Based on low heating value of a fuel, an HICE emits nearly three times as much water per energy content, compared to a conventional ICE which runs on gasoline. The stoichiometric heat of combustion values per standard kg of air are 3.37 MJ and 2.83 MJ for hydrogen and gasoline, respectively [11]. The adiabatic flame temperature calculated value using the Adiabatic Flame Temperature Program developed by C. Depcik [12] showed that the combustion temperature of hydrogen fuel was approximately 126^{a}C higher than that of gasoline fuel, when the combustion process occurred at A = 1. Therefore, an HICE is expected to have a high temperature level for its waste heat and there is a potential that the heat can be utilized in many ways.

In addition, the greatest issue for spark-ignited HICE combustion is the occurrence of a backfire and/or pre-ignition as the lean fuel/air ratio approaches the stoichiometric value, which

[2] Large amount of water also compared to the fuel cells, and the detail calculation relating to the water amount from HICE, ICE and FC shown in Appendix 1.

limits the torque output of the engine [8]. The HICE power density, relative to gasoline operation, can be significantly below 83%, due to pre-ignition problems limiting the peak power output of the HICE [11]. Tang et al. (2002) [8] and Furuhama et al. (1978) [13] reported that pre-ignition ignition limited the power density to 50% and 72%, respectively, relative to gasoline operation. A backfire occurs when a fresh charge of hydrogen is ignited in the intake ports, while pre-ignition occurs when the hydrogen charge is ignited after the intake valve closes but before the spark plug fires in the cylinder [14]. Both problems can be caused by the existence of a high temperature spot in the intake manifold or cylinder [11, 14].

Inspired from the above-mentioned aspects of an HICE, a new concept for a recovery sub-system that uses both the waste heat and water emitted from an HICE, to enhance its thermal efficiency has been proposed. The proposed sub-system is expected to mitigate the high temperature spot problem by absorbing the undesirable excess heat from the HICE.

The following equation shows the HICE combustion process [15]:

$$2H_2 + \lambda \cdot O_2 + 3.76 \cdot \lambda \cdot N_2 \rightarrow 2H_2O + (\lambda - 1) \cdot O_2 + 3.76 \cdot \lambda \cdot N_2 \quad (1)$$

where λ denotes the ratio of the actual air quantity to the theoretical demand. The emissions produced by the HICE are, theoretically, only water and nitrogen gas when combustion is ideally carried out at a stoichiometric air-fuel ratio (AFR) of 34:1 with $\lambda = 1$, and other factors such as oxidation of the lubrication oil or the existence of other gases in the air are neglected. From Eq. (1), it is found that when 1 kg of hydrogen mass is supplied to the engine, approximately 9 kg of water are generated chemically by the combustion process at $\lambda = 1$. This seems to be enough water for the open steam Rankine cycle, which releases the water to the outside atmosphere after it is used to produce power. In an actual case, the air supplied to the HICE is humid; that is, the supplied air includes water vapor. Theil and Hartmann (2008) [16] of BMW reported detailed emissions data for an HICE using the hydrogen-balance method. From their results, it was estimated that the amount of water vapor emitted by the HICE was approximately 8.9 kg for 1 kg of hydrogen combusted for an actual driving distance of 100 km.

In addition, it is not always beneficial to have a large amount of water in the exhaust, since it affects, not only the exhaust system, but also any additional devices installed in, the exhaust system. It is known that water vapor accelerates the corrosion of an exhaust pipe under a high temperature condition, which causes the carbon monoxide (CO) and carbon dioxide ($C0_2$) detectors to provide incorrect readings. Therefore, removing the water from the exhaust may contribute to the mitigation of these problems.

1.2 Research background

Recently, the worldwide energy crisis and environmental issues have prompted vehicle manufacturers to produce vehicles with high energy efficiency using power generation processes that do not harm the environment. In the case of conventional internal combustion engines (ICEs), many studies on waste heat recovery sub-systems have been conducted to enhance the overall thermal efficiency. One of the most frequently used recovery sub-systems for automobile application is a Rankine cycle, i.e., a steam power generation cycle [17-20], and also organic Rankine cycle (ORC) [18, 21-23]. There are two types of Rankine cycles: a closed Rankine cycle and open Rankine cycle. In an open Rankine cycle system, the working fluid is ejected from the system after it produces work output, while it is reused in the closed cycle. A classical locomotive steam engine is an example of a successful open Rankine cycle system. Although there are many types of working fluids for the Rankine cycle, water is one of the most desirable fluids in terms of safety, environmental friendliness, and thermodynamic characteristics at high temperatures and pressures [17].

Although there are possibility to improve the thermal efficiency of conventional ICEs through the adaptation of waste heat recovery sub-systems, the ICE's operation based on carbon containing fuels (including Diesel engine) itself is actually a major contributor to the production of green house gas (as mentioned in previous sub-section) . Since the future prospect of the conventional ICEs is not so attractive, the introduction of HICE will not only ensure,the continuation of ICE's life, but the HICE also represent a countermeasure for ICEs operation to reduce the environmental impact. HICE also considered to be a cost competitive and clean compared to the conventional ICEs [24], and offers the potential to contribute to the reduction of green house gases and local air pollution [25] (as discussed in previous sub-section). Therefore, it would be considered as a promising candidate for future automobile power train system alternative to conventional ICEs. In consequence, this reflects the future target of introducing the recovery sub-system into ICEs, that should be reconsidered by redirect the target to the HICE.

The two important aspects of HICE as mentioned earlier, i.e., high amount of waste heat, and water as a by-product of combustion, should not be abandoned but positively view both of the aspects as valuable sources. The waste heat from HICE in this case should be treated as low-grade heat that capable of producing the useful energy through heat recovery sub-system, whereas the water would be a potentially valuable resource if it could be utilized for some useful purpose such as for the working fluid in a heat recovery system. For a power plant system, Sugisita et al. (1998) [26] reported simulation results for a closed hydrogen combustion turbine cycle that was powered by extracted steam from hydrogen combustion combined with a closed Rankine cycle as a bottoming cycle. Thus far, however, no research has been conducted on a recovery sub-system that recovers both waste heat and water from an HICE, especially in an automotive application.

Inspired by the potential of HICE to be a future automobile power train system, and both HICE waste heat and water, a new concept for a recovery sub-system for an HICE based on open steam Rankine cycle will be proposed for an HICE in automobile application. The recovery sub-system is expected to exploit the water emitted from the HICE as its working fluid, and convert the waste heat from the HICE into power. As a result, the net power and thermal efficiency produced by the HICE combined with the recovery sub-system are expected higher than that produced by the HICE alone.

1.3 Research objective and scope

According to the potential of HICE to be a future automobile power train system, the drawback effects of the high amount of heat and water produced by the HICE, and the motivation of the recovery sub-system which is capable to enhance the thermal efficiency of HICE, the aim of this study is to describe and simulate a new concept of the recovery sub-system (i.e., recovering both waste heat and water) from HICE in an automotive application. Then, the most potential recovery sub-system will be proposed to be adopted into the real automobile HICE, based on it's the performance evaluation, design practicality and cost factor. Two designs of the fundamental thermodynamic model (i.e., steam Rankine cycle); one with a condenser and another one without the condenser, for the recovery sub-system will be examined, and the thermal efficiency of the single recovery sub-system and the overall thermal efficiency of the entire system[3] will be estimated under various engine speed conditions for the HICE.

The scope of this study is limited to the first order simulation based on fundamental thermodynamic analysis for both of the recovery sub-system models. Most of the HICE data used in this based on available published data from the other research. Reasonable assumptions will be used during the simulation for deciding the HICE and recovery sub-systems conditions, which are absence in the literatures. The HICE condition chosen in this study is limited to the engine speed ranges within 1500 to 4500 rpm, running at fixed torque of 40 Nm.

[3] Combined HICE and recovery sub-system.

1.4 Thesis layout

The details work carried out relating to this study will be described in five chapters. The outline of this thesis is summarily described as follows:-

Chapter 1 - Highlights the benefits of using hydrogen as fuel and the prospect of HICE as future automobile power train system, briefly describes the HICE behaviors relating to this research, some important research background, and the objectives and scopes of this research. .

Chapter 2 - Describes the recovery sub-system for automobile HICE; a general steam Rankine will firstly introduced followed by description given for both designs of the recovery sub-system chosen in this study.

Chapter 3 - This is the main part of the dissertation that shows the simulation model and method: it highlights the models, the fundamental equations used both for HICE and recovery sub-systems, and the method used to simulate for different conditions.

Chapter 4 - Presents the simulation results and discussion: the result of each recovery sub-system and the combined system is firstly showed separately, then their performance is reviewed as a whole. The sufficient amount of water as working fluid, and some factors attributed to the increase and reduction of overall system performance are also clarified.

Chapter 5 - Summarizes the findings and results of this work, and suggests for the future work related to this research.

Chapter 2

Recovery sub-system

2.1 Overview of Rankine cycle

Rankine cycle (also called ideal vapor power cycle) is a modified Carnot cycle to overcome many of the impracticalities associated with the Carnot cycle, when the working fluid is vapor [2, 27]. It owns about similar behavior to Carnot cycle especially during isothermal heat transfer processes, i.e., condensation and evaporation [27]. In Rankine cycle, the working fluid is alternately condensed and vaporized, and its temperature is constant when it remains in the saturation region at constant pressure. In the Rankine cycle, the heating and cooling processes occur at constant pressure, and for an ideal Rankine cycle, it does not involve any internal irreversibilities. Fig. 1(a) shows the configuration of a basic Rankine cycle, and Fig. 1(b) is the temperature-entropy (T-s) diagram of the basic Rankine cycle (ideal).

There are four basic process of an ideal Rankine cycle, process 1-2: isentropic compression in a pump (external work required), 2-3: constant pressure heat addition in a boiler, 3-4: isentropic expansion in a turbine (work produced) and 4-1: constant pressure heat rejection in a condenser.

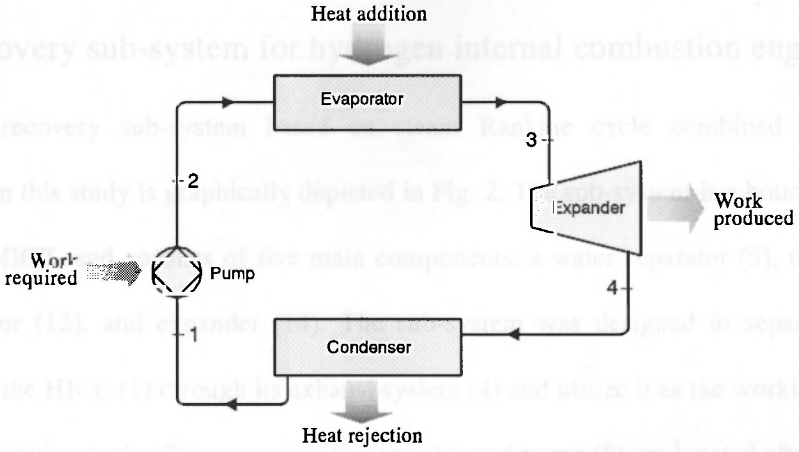


Fig. 1(a) – Configuration of basic Rankine cycle

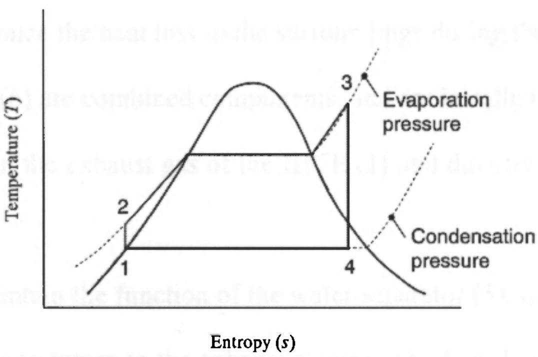


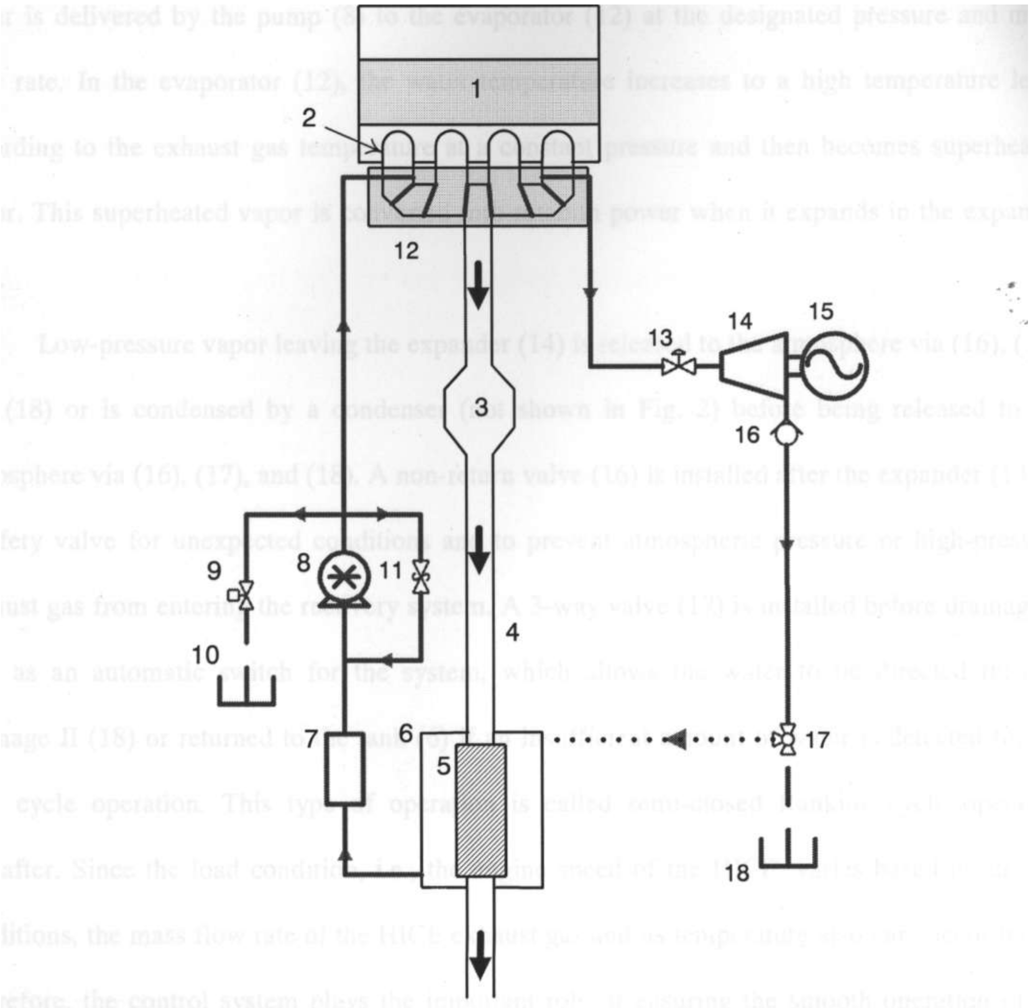
Fig. 1(b) – *T-s* diagram of basic Rankine cycle (ideal)

Unlike the ideal Rankine cycle, an actual Rankine cycle operates differently with the internal irreversibilities occur in almost all in its components. Almost all of the present Rankine cycles developed or investigated by other researchers faced the irreversibilities problem, and there is no ideal Rankine cycle has been successfully produced by anyone, due to difficulty or limitations to provide the ideal components for the cycle. In this study, an actual Rankine cycle is chosen as the recovery sub-system for HICE. The components irreversibilities are given (i.e., in the form of their efficiencies) to the recovery sub-system design in order to simulate as closed as possible to an actual and practical system.

2.2 Recovery sub-system for hydrogen internal combustion engine

The recovery sub-system based on steam Rankine cycle combined to the HICE investigated in this study is graphically depicted in Fig. 2. The sub-system is a bottoming cycle of the primary HICE, and consists of five main components: a water separator (5), tank (6), pump (8), evaporator (12), and expander (14). The sub-system was designed to separate the water emitted from the HICE (1) through its exhaust system (4) and utilize it as the working fluid of the open steam Rankine cycle. The separator (5), tank (6), and pump (8) are located after the catalytic converter (3) of the HICE, whereas the evaporator (12) is located on the exhaust manifold in order to extract high temperature waste heat. The expander (14) is located as close as possible to the evaporator to minimize the heat loss to the surroundings during the cycle operation. The water separator (5) and tank (6) are combined components, and are installed in the exhaust system (4) to separate the water from the exhaust gas of the HICE (1) and directly store the separated water in the tank (6).

In order to maintain the function of the water separator (5), the separated water inside the tank should not be able to return to the exhaust system, which will continuously add water to the tank (6). A water filter (7) is installed before the pump (8) to remove contaminants from the separated water in the tank, because the untreated water inside the tank may contain contaminants in the form of gases, hydrocarbons, particulates, and other dissolved organic and inorganic matter. Since the water is continuously supplied to the recovery sub-system, there should be a mechanism to control the water level inside the tank, so that the amount of water is always at an optimum level. This can be done by a control system (not shown in Fig. 2) that allows any excess water to be drained to the atmosphere through drainage I (10). Here, power valve I (9) automatically opens and closes the drainage line based on the water level in the tank. A relief valve (11) is installed in parallel with the pump (8) to maintain the system pressure under the allowable pressure level. The



Component Description

1. HICE
2. Exhaust Manifold
3. Catalytic Converter
4. Exhaust Waste
5. Water Separator
6. Tank
7. Water Filter
8. Pump
9. Power Valve
10. Drainage 1
11. Relief Valve
12. Evaporator
13. Adjustable Valve
14. Expander
15. Electric Generator
16. Non-return Valve
17. 3-Way Valve
18. Drainage II

Line and Shape Description

•	Exhaust Flow
_ . _	Flow Direction
. . . > —	Return Line

Fig. 2 - HICE system combined with open steam Rankine cycle recovery sub-system

The power produced by the expander (14) is used to drive an electrical generator (15). The generated electric power could be utilized in many ways, such as being directed to a battery, driving electrical devices, or for other purposes. The separation of water from the exhaust gas in the water separator (5) is one of key processes of the proposed sub-system. However, the design details for this water separator were not discussed in this study. Interesting designs for water separators have recently been proposed by some inventors [28-30]. One example is the inertial water separator. In this study, it was assumed that the water separator performs its separation with an efficiency of 50%, as mentioned later, and that the water separator does not consume power.

Chapter 3

Simulation model and method

The objectives of the present simulation were to elucidate the thermal efficiency of the recovery sub-system, to show whether the recovery sub-system has the potential to contribute to the overall thermal efficiency of the entire system, and to determine whether a sufficient amount of working fluid (water) could be recovered by the water separator to recover the heat wasted through the HICE exhaust system.

Fig. 3 shows a simulation model of the open steam Rankine cycle recovery sub-system. The layout of the main components is similar to Fig. 2 and each link between the components is marked with a number representing the state of the working fluid. Here, the condenser and electric fan inside the enclosed dashed-dotted line represent an optional configuration for recovery sub-system II (RS-II). The electric fan is incorporated with the condenser to enhance the heat transfer from the condenser to the ambient air. The system without the condenser is hereafter called recovery sub-system I (RS-I), whereas the system with the condenser (and electric fan) is called RS-II. The solid line with the arrows in Fig. 3 represents the flow direction of the working fluid for RS-I, whereas the dashed line represents the flow direction modification for RS-II. The working fluid in RS-II flows through the dashed line into the condenser before it

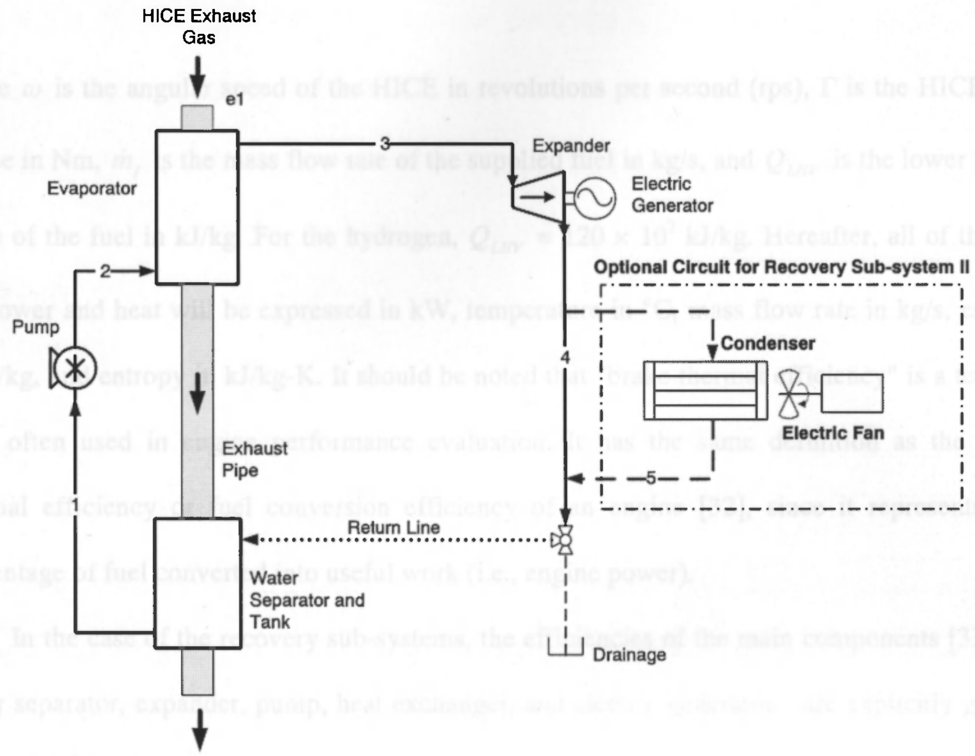


Fig. 3 – Simulation model of open steam Rankine cycle recovery sub-system

is drained or directed to the tank. The condenser in RS–II was installed to elucidate its effect on the thermal efficiency of the recovery sub-system and the overall thermal efficiency of the entire system since a condenser is generally employed in a conventional closed steam Rankine cycle to reduce the pressure at the expander outlet, and to increase the thermal efficiency of the cycle.

In this study, the HICE conditions, engine power, total combustion heat, and brake thermal efficiency of the engine, were calculated as follows [31, 32]:

$$W_{HICE} = 2 \cdot \pi \cdot \omega \cdot \Gamma \times 10^{-3} \tag{2}$$

$$Q_{total} = \dot{m}_f \cdot Q_{LHV} \tag{3}$$

$$\eta_{BTE} = \frac{W_{HICE}}{Q_{total}} = \frac{W_{HICE}}{\dot{m}_f \cdot Q_{LHV}} \tag{4}$$

where ω is the angular speed of the HICE in revolutions per second (rps), Γ is the HICE brake torque in Nm, $\dot{m}_f$ is the mass flow rate of the supplied fuel in kg/s, and Q_{LHV} is the lower heating value of the fuel in kJ/kg. For the hydrogen, Q_{LHV} = 120 × 10^3 kJ/kg. Hereafter, all of the units for power and heat will be expressed in kW, temperature in °C, mass flow rate in kg/s, enthalpy in kJ/kg, and entropy in kJ/kg-K. It should be noted that "brake thermal efficiency" is a technical term often used in engine performance evaluation. It has the same definition as the overall thermal efficiency or fuel conversion efficiency of an engine [32], since it represents some percentage of fuel converted into useful work (i.e., engine power).

In the case of the recovery sub-systems, the efficiencies of the main components [33]—the water separator, expander, pump, heat exchanger, and electric generator—are explicitly given as shown in Table 2.

Table 2 – Efficiencies for recovery sub-system components.

Component	Efficiency
Water separator[a]	η_S = 50%
Pump[b]	η_P = 60%
Expander[b]	η_E = 70%
Electric generator[a]	η_G = 85%
Heat exchanger[a]	η_{HX} = 80%

[a] Estimated data.
[b] Data was taken from Chammas and Clodic (2005).

For the separation process, the water separator efficiency is defined by the following equation:

$$\eta_S = \frac{\dot{m}_{sw}}{\dot{m}_T} \tag{5}$$

where $\dot{m}_{sw}$ is the mass flow rate of the separated water and $\dot{m}_T$ is the mass flow rate of the total amount of water in the HICE exhaust gas before the separation process. The efficiencies of the expander and pump are defined as:

$$\eta_E = \frac{h_3 - h_{4a}}{h_3 - h_{4s}} \tag{6}$$

$$\eta_P = \frac{h_{2s} - h_1}{h_{2a} - h_1}, \tag{7}$$

respectively, where h is the enthalpy of the working fluid. The subscripts a and s for the enthalpy refer to actual (non-isentropic) and ideal (isentropic) processes, respectively. The subscript numbers correspond to the numbers in Fig. 3. The electric generator efficiency is defined as:

$$\eta_G = \frac{W_G}{W_E} \tag{8}$$

where W_G is the generated electric power and W_E is the power converted by the expander. When the heat loss from the heat exchanger to the surroundings is negligible, the performance of heat exchanger is represented by its effectiveness. The effectiveness is defined as the ratio of the actual rate of heat transfer by the heat exchanger to the maximum possible heat transfer rate between the fluids [34-37]. Therefore, in this study the heat exchanger effectiveness is given as

$$\varepsilon = \frac{T_3 - T_{2a}}{T_{e1} - T_{2a}} \tag{9}$$

where ε is the heat exchanger effectiveness and ε = 0.8 is assumed in the simulation. T_{e1} is the temperature of the HICE exhaust gas entering the evaporator, whereas T_{2a} and T_3 are the temperature of water at evaporator inlet and outlet, respectively. The energy balance in the evaporator is conserved by the following equations:

$$Q_{evap} = Q_{exh} - Q_{ew} \tag{10}$$

$$Q_{evap} = \frac{Q_{in}}{\eta_{HX}} = \frac{\dot{m}_w (h_3 - h_{2a})}{\eta_{HX}} \tag{11}$$

where Q_{evap} is the portion of the HICE exhaust waste heat that passes through the evaporator and is used as a heat source for the recovery sub-system, $\dot{m}_w$ is the mass flow rate of the working fluid (water) controlled by the pump, η_{HX} is the heat exchange efficiency of the evaporator, Q_{in} is the heat that the working fluid gains at the evaporator, Q_{exh} is the HICE exhaust waste heat (i.e., the heat of the HICE exhaust gas), and Q_{ew} is the heat leaving the HICE exhaust gas before the gas reaches the evaporator. In this study, Q_{ew} = 0.2 × Q_{exh} is assumed.

The generated electric power is calculated as:

$$W_G = \dot{m}_w \eta_G (h_3 - h_{4a}) \ . \tag{12}$$

The pump power is calculated as:

$$W_P = \dot{m}_w (h_{2a} - h_1) \tag{13}$$

The net thermal efficiencies of RS–I and RS–II can then be calculated using:

$$\eta_{th} = \frac{W_G - W_P}{Q_{in}} \tag{14}$$

The net power values for RS–I and RS–II are respectively defined as follows:

$$W_{RS\text{-}I} = W_G - W_P \tag{15}$$

$$W_{RS\text{-}II} = W_G - W_P - W_C \tag{16}$$

where W_C is the electric power consumption of the electric fan incorporated with the condenser (hereafter, W_C is called "condenser fan power") in RS–II. Finally, the total power and overall thermal efficiency of the entire system are given by:

$$W_{total} = W_{HICE} + W_{RS\text{-}I}, \quad \text{or} \quad W_{total} = W_{HICE} + W_{RS\text{-}II} \tag{17}$$

$$\eta_{overall} = \frac{W_{total}}{Q_{total}} \tag{18}$$

where Q_{total} is the total heat provided by the hydrogen combustion in the HICE, as defined by Eq. (3).

The simulation work in this study began by analyzing the HICE conditions by extracting the engine parameters from the available published data on HICEs. Verhelst et al. [38] reported that a four-cylinder sixteen-valve engine with a displacement volume of 1783 cc, running on hydrogen fuel, has brake thermal efficiencies, η_{BTE}, that are relatively higher than when it runs on gasoline fuel at a specific brake torque, Γ. Table 3 shows the selected engine experimental conditions for this study taken from their experiments. Based on their data for the η_{BTE} at Γ = 40 Nm, with an engine running on hydrogen fuel under stoichiometric conditions, the W_{HICE} and $\dot{m}_f$

values can be estimated using Eqs. (2) and (4), respectively, at various engine speeds. From Eq. (3), Q_{total} can be estimated after the value of $\dot{m}_f$ is known. Due to the absence of available data for the heat balance of an HICE, the Q_{exh} of the HICE was assumed from the data for a gasoline/hydrogen mixed fuel engine [39]. Yüksel and Ceviz observed that the heat loss through the exhaust gas of a four-cylinder engine with a 1796 cc displacement volume burning a gasoline/hydrogen mixed fuel was nearly the same as when it operated on pure gasoline. Based on their percentage value data for the heat loss through the exhaust gases at various engine speeds, the same percentage was assumed for Q_{exh} in this study. The selected engine experimental conditions for this analysis taken from their experiment are shown in Table 4. The other energy fractions, i.e., Q_{total} and W_{HICE}, were taken directly from the Verhelst et al. [38] study, whereas the other unspecified energy fraction (consisting of cooling and other losses) was estimated by subtracting all of the known energy fractions from Q_{total}. Fig. 4 shows the HICE energy fractions, which included the HICE exhaust waste heat Q_{exh}, engine power W_{HICE}, and other unspecified heat losses (these are called "HICE cooling and other losses" hereafter).

Table 3 – Selected engine condition taken from experiment by Verhelst et al. [38].

Engine experimental condition	Data
Engine type	Volvo (with CVVT), fuel injected
Fuel used	Hydrogen
Number of cylinders	4
Compression ratio	10.3 : 1
Displacement volume	1783 cc
Air fuel ratio, λ	1 (fixed)
Engine brake torque, Γ	40 Nm (fixed)
Engine speed	1500 ~ 4500 rpm

Table 4 – Selected engine condition taken from experiment by Yüksel and Ceviz [39].

Engine experimental condition	Data
Engine type	Ford MVH-418, fuel injected
Fuel used	Hydrogen – gasoline (mixed)
Number of cylinders	4
Compression ratio	10 : 1
Displacement volume	1796 cc
Air fuel ratio, λ	1.0 ~ 0.8 (varies)
Engine brake torque, Γ	100 ~ 157 Nm (varies)
Engine speed	1500 ~ 4500 rpm

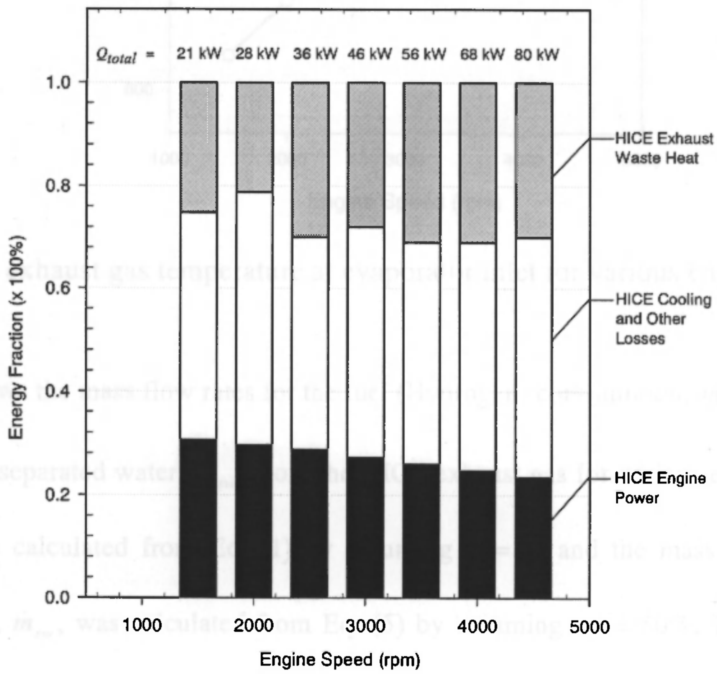


Fig. 4 – Energy fractions of HICE without recovery sub-systems for various engine speeds [38, 39]

Fig. 5 shows the exhaust gas temperatures of the HICE at the evaporator inlet and outlet for various engine speeds. The data for the HICE exhaust gas temperatures at the exhaust manifold, T_{e1}, reported by Verhelst et al. [38] at 3500 rpm and 4500 rpm were used. Based on their data, the temperature variation was assumed to be linear with the engine speed. The recovery sub-system was assumed to be ideally insulated, so that there was no heat loss through the system boundaries, such as pipes, component walls, etc.

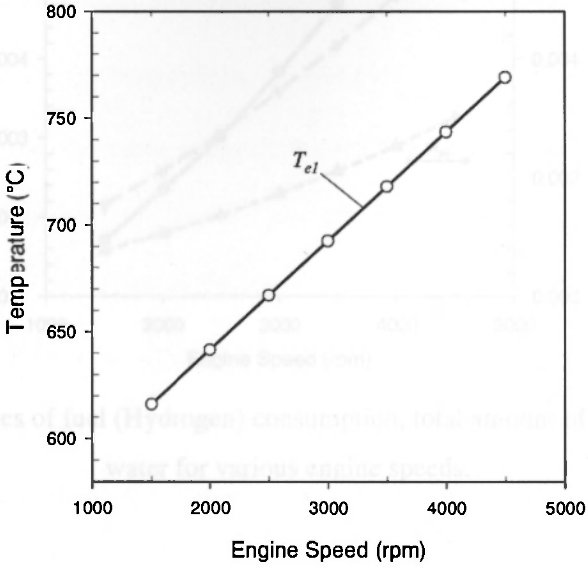


Fig. 5 – HICE exhaust gas temperature at evaporator inlet for various engine speeds [38]

Fig. 6 shows the mass flow rates for the fuel (Hydrogen) consumption, $\dot{m}_f$, total amount of water, $\dot{m}_T$, and separated water, $\dot{m}_{sw}$, from the HICE exhaust gas for various engine speeds. The $\dot{m}_T$ values were calculated from Eq. (1) by assuming λ = 1, and the mass flow rate for the separated water, $\dot{m}_{sw}$, was calculated from Eq. (5) by assuming η_S = 50%. The required mass flow rate of the working fluid water, $\dot{m}_w$, varied with the engine speed ($\dot{m}_w$ is shown in Fig. 10). For continuous operation of the proposed sub-system, the value of $\dot{m}_w$ should be less than that of $\dot{m}_{sw}$ in the case without the semi-closed Rankine cycle operation (i.e., open steam Rankine cycle operation).

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