UNIVERSITI PUTRA MALAYSIA

GENERATING POWER FROM FLUEGAS PRODUCED BY BOILERS THROUGH THERMODYNAMIC ORGANIC RANKINE CYCLE

OMID ROWSHANAIE

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GENERATING POWER FROM FLUEGAS PRODUCED BY BOILERS THROUGH THERMODYNAMIC ORGANIC RANKINE CYCLE

By

OMID ROWSHANAIE

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirement for the Degree of Master of Science

September 2015

DEDICATION

This thesis is dedicated to

My merciful father,

my sympathetic mother, and

my only brother.

for their endless love, support and encouragement

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the Degree of Master of Science

GENERATING POWER FROM FLUEGAS PRODUCED BY BOILERS THROUGH THERMODYNAMIC ORGANIC RANKINE CYCLE

By

OMID ROWSHANAIE

September 2015

Chairman : Associate Professor Saari Mustapha, Ph.D.
Faculty : Engineering

A simulation model of Organic Rankine Cycle (ORC) was developed with HYSYS simulation software driven by R245fa, with NOVEC7000 and R141b as refrigerant working fluids and wet fluegas combustion and burning from natural gas, as a heat source of shell and tube heat exchanger to generate optimum power by an expander (more than 3MW that proper amount of energy for applying in refinery and petrochemical industries). The initial operating conditions were in subcooled liquid, normal, and steady state condition. In current ORC, refrigerant working fluids were sent to a heat exchanger to change the phase fraction from 0 to 1, then input to an expander to produce optimum power. However, the changing of all parameters were affected by different mass flow rates of working fluids and different inlet pressures of expander. The ORC thermodynamic cycle was chosen for this study due to some advantages such as its simple structure, the availability of its components, and the ease of application for small and optimum industrial power generation.

Regarding to current study results, different mass flow rates of working fluids and different inlet pressures of expander had linear relationship with power output from the expander. Therefore, R141b was found to be produced the highest power output from the expander up to 13520 KW, compared to NOVEC7000 where by the power being produced 35 % less and the lowest power generated by the expander belonged to R245fa refrigerant with 53 % reduction. Also the highest net power generated output from the ORC was from R141b which the highest power was 12194 KW, followed by NOVEC7000 and R245fa gave as the lowest net power output, 37 % and 57 % reduction respectively. For the heat transfer from the fluegas to the working fluid ascendancy; R141b with 3.780×10^9 kJ/h, then R245fa 18 % less and NOVEC7000 38 % reduction respectively.

Furthermore, in terms of total efficiency of ORC depend on different inlet pressures of expander, NOVEC7000 was chosen as highest total efficiency with 90.8 % and R141b was chosen as middle total efficiency with 90.6 % were the suitable options compare with R245fa which value was i.e. 85.0 % the lowest total efficiency of ORC. The thermal efficiency of the ORC for different mass flow rates of working fluids and different inlet pressures of expander were analyzed and there were no

remarkable differences between R245fa, NOVEC7000, and R141b. The polytropic efficiency of the expander was evaluated at different specific pressures of each working fluid at the inlet of expander. The result was indicated NOVEC7000 superior in which it given 80.3 % of the polytropic efficiency followed by R141b and R245fa with 70.5 % and 40.1 % respectively. On the other hand, no remarkable difference of the exergy efficiency for the ORC at maximum total irreversibility and maximum heat exchanger exergy of present ORC.

Abstrak tesis dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

MENJANA KUASA DARI FLUEGAS DIHASILKAN OLEH PENDIDIHAN MELALUI ORGANIC RANKINE CYCLE TERMODINAMIK

Oleh

OMID ROWSHANAIE

September 2015

Pengerusi : Prof Madya Saari Mustapha, Ph.D.
Fakulti : Kejuruteraan

Satu model simulasi ORC telah dihasilkan dengan menggunakan perisian simulasi HYSYS dengan bantuan oleh R245fa, manakala NOVEC7000 dan R141b yang bertindak sebagai penyejuk bendalir kerja dan pembakaran *fluegas* basah dan pembakaran dari gas semulajadi, sebagai punca haba untuk penukar haba jenis *cengkerang dan tiub* bagi menghasilkan kuasa optimum daripada *expander* (3 MW adalah nilai tenaga yang sesuai digunakan dalam industri penapisan dan Petrokimia). Keadaan permulaan operasi adalah di dalam bentuk cecair separasejuk, normal dan stabil. Dalam keadaan ORC terkini, penyejuk bendalir kerja dihantar ke penukar haba bagi menukar pecahan fasa dari 0 ke 1, kemudian input kepada *expander* untuk menghasilkan kuasa optimum. Walau bagaimanapun perubahan kesemua paramater adalah dipengaruhi oleh kadar aliran jisim dan perubahan tekanan masuk *expander*. Kitaran Thermodinamik ORC dipilih untuk kajian ini adalah berdasarkan kepada beberapa kelebihan seperti strukturnya yang ringkas, kebolehdapatan bagi setiap komponen dan kemudahan aplikasi untuk generasi industri kuasa yang kecil dan optimum. Berdasarkan dari hasil kajian terkini menunjukkan bahawa perbezaan kadar aliran jisim sesuatu bendalir kerja dan perbezaan tekanan masuk *expander* mempunyai hubungan yang linear kepada kuasa *output* daripada *expander*. Oleh sebab itu, R141b didapati telah menghasilkan kuasa output paling tinggi daripada expander sehingga mencecah kepada 13520 KW, dibandingkan dengan NOVEC7000 dimana kuasa expander yang dihasilkan adalah 35% kurang dan kuasa yang terendah yang dihasilkan daripada expander penyejuk R245fa adalah pengurangan sebanyak 53%. Kuasa bersih yang dihasilkan daripada output ORC R141b adalah yang tertinggi iaitu sebanyak 12194KW, diikuti oleh NOVEC7000 dan R245fa memberikan nilai terendah bagi kuasa output, masing-masing dengan pengurangan 37% dan 57% . Untuk pemindahan haba daripada *fluegas* kepada *kekuasaan* bendalir kerja: R141b dengan 3.780×10^{9} kJ/h, kemudian R245fa berkurangan 18% dan NOVEC7000 berkurangan 38%.

Selain itu, dari segi jumlah kecekapan ORC adalah bergantung kepada perubahan tekanan masuk *expander*. NOVEC7000 telah terpilih sebagai jumlah kecekapan tertinggi dengan 90.8% dan R141b pula terpilih sebagai pertengahan jumlah kecekapan dengan nilai 90.6%. Nilai ini adalah pilihan yang sesuai jika dibandingkan

dengan R245fa yang nilainya adalah yang paling rendah bagi ORC iaitu sebanyak 85.0%. Jumlah kecekapan thermal bagi ORC untuk perbezaan kadar aliran jisim bagi bendalir kerja dan perbezaan tekanan masuk *expander* telah dianalisis dan tiada perbezaan yang ketara diantara R245fa, NOVEC7000 and R141b. Kecekapan *Polytropic expander* dinilai berdasarkan perbezaan tekanan tertentu untuk setiap bendalir kerja di tempat masuk *expander*. Keputusan ini menunjukkan NOVEC7000 adalah yang terbaik dengan 80.3% kecekapan *polytropic*, diikuti dengan R141b and R245fa dengan masing-masing 70.5% and 40.1%. Sebaliknya, tiada perubahan ketara untuk kecekapan *exergy* bagi ORC pada jumlah tidak boleh mengembalikan kuasa maksimum dan penukar haba *exergy* maksimum bagi ORC masa kini.

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I certify that a Thesis Examination Committee has met on 21 September 2015 to conduct the final examination of Omid Rowshanaie on his thesis entitled "Generating Power from Fluegas Produced by Boilers Through a Thermodynamic Organic Rankine Cycle" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 march 1998. The Committee recommends that the student be awarded the Master of Science.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfillment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

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Declaration by Members of Supervisory Committee

This is to confirm that:

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Signature: ________________________
Name of Chairman of Supervisory Committee: Sa'ari Bin Mustapha, PhD

Signature: ________________________
Name of Member of Supervisory Committee: Kamarul Arifin Ahmad, PhD

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Symbol	Quantity	Unit
ORC	Organic Rankine Cycle	-
Δh_{vap}	Heat of vaporization	(kJ/kg)
ρ_{vap}	Density in vapor state	(kg/m^3)
$m_{M.W}$	Molecular weight	(kg/mole)
$T_{b,p}$	Boiling point temperature	($^\circ C$)
$\rho_{I.L}$	Ideal liquid density	(kg/m^3)
T_c	Critical temperature	($^\circ C$)
P_c	Critical pressure	(KPa)
V_c	Critical volume	(m^3)
F_t	LMTD correction factor	-
$dt_{hot\ end}$	Temperature difference at the outlet of heat exchanger (hot area)	($^\circ C$)
$dt_{cold\ end}$	Value of heat transfer between fluegas to working fluid (cold area)	($^\circ C$)
U	Overall heat transfer capacity of heat exchanger	($KW/^\circ C$)
$\Delta T_{pinch\ H.E\ (R245fa)}$	The pinch temperature difference in shell and tube heat exchanger for R245fa	($^\circ C$)
$\Delta T_{pinch\ cooler\ (R245fa)}$	The pinch temperature difference in cooler for R245fa	($^\circ C$)
$\Delta T_{pinch\ H.E\ (NOVEC7000)}$	The pinch temperature difference in Shell and Tube heat exchanger for NOVEC7000	($^\circ C$)
$\Delta T_{pinch\ cooler\ (NOVEC7000)}$	The pinch temperature difference in cooler for NOVEC7000	($^\circ C$)
$\Delta T_{pinch\ H.E\ (R141b)}$	The pinch temperature difference in Shell and Tube heat exchanger for R141b	($^\circ C$)
$\Delta T_{pinch\ cooler\ (R141b)}$	The pinch temperature difference in cooler for R141b	($^\circ C$)
$\dot{W}_{net}$	Maximal net power output of ORC	(KW)
$\dot{W}_{Ex}$	Net power output of expander	(KW)
$\dot{W}_{cooler}$	Power generated by the cooler	(KW)
$\dot{W}_{Pump}$	Power consumed by the pump	(KW)
$\dot{Q}_{H.E}$	Heat transfer from fluegas to working fluid (heat rate injected)	(kJ/h)
$\dot{m}_{ORC}$	Mass flow rate of each working fluids	(kg/h)
$h_{outlet\ of\ H.E}$	Enthalpy at outlet of heat exchanger	(kJ/kg)
$h_{inlet\ of\ H.E}$	Enthalpy at inlet of heat exchanger	(kJ/kg)
$(UA)_{total}$	Total heat transfer capacity	($KW/^\circ C$)
$\Delta T_{H.E}$	Maximal and minimal temperature differences at the tube and shell heat exchanger	($^\circ C$)
$\dot{Q}_{cooler}$	heat rate rejected	(kJ/h)
$\dot{m}_{W.F}$	Mass flow rate of working fluids	(kg/h)
h_{outlet}	Outlet Enthalpy	(kJ/kg)
h_{inlet}	Inlet Enthalpy	(kJ/kg)

T_{inlet}	Inlet temperature	(°C)
T_{outlet}	Outlet temperature	(°C)
I_{pump}	Irreversibility of pump	(KW)
$I_{H.E}$	Irreversibility of shell and tube heat exchanger	(KW)
I_{Ex}	Irreversibility of expander	(KW)
I_{cooler}	Irreversibility of cooler	(KW)
I_{total}	Total Irreversibility of ORC	(KW)
T_0	Dead-state temperature	(°C)
$S_{outlet\ of\ pump}$	Mass entropy at outlet of pump	(kJ/kg °C)
$S_{inlet\ of\ pump}$	mass entropy at inlet of pump	(kJ/kg °C)
$S_{outlet\ of\ H.E}$	Mass entropy at outlet of shell and tube heat exchanger	(kJ/kg °C)
$S_{inlet\ of\ H.E}$	Mass entropy at inlet of shell and tube heat exchanger	(kJ/kg °C)
$S_{fluegas\ out}$	Mass entropy at outlet of fluegas	(kJ/kg °C)
$S_{fluegas\ in}$	Mass entropy at inlet of fluegas	(kJ/kg °C)
$h_{inlet\ of\ Ex}$	enthalpy at inlet of expander	(kJ/kg)
$h_{outlet\ of\ Ex}$	enthalpy at outlet of expander	(kJ/kg)
$S_{inlet\ of\ cooler}$	Mass entropy at inlet of cooler	(kJ/kg °C)
$S_{outlet\ of\ cooler}$	Mass entropy at outlet of cooler	(kJ/kg °C)
$E_{H.E}$	exergy of heat exchanger	(KW)
E_{cooler}	exergy ofc	(KW)
$E_{fluegas}$	exergy of fluegas	(KW)
E_{total}	Total exergy of ORC	(KW)
$h_{outlet\ of\ H.E}$	enthalpy at outlet of heat exchanger	(kJ/kg)
$h_{inlet\ of\ H.E}$	enthalpy at inlet of heat exchanger	(kJ/kg)
$h_{inlet\ of\ cooler}$	enthalpy at inlet of cooler	(kJ/kg)
$h_{outlet\ of\ cooler}$	enthalpy at outlet of cooler	(kJ/kg)
$h_{fluegas\ in}$	enthalpy at inlet of fluegas	(kJ/kg)
$h_{fluegas\ out}$	enthalpy at outlet of fluegas	(kJ/kg)
$T_{outlet\ of\ H.E}$	Absolute temperature at which heat is absorbed (it means at the outlet of heat exchanger)	(°C)
$T_{outlet\ of\ cooler}$	Absolute temperature at which heat is rejected (it means at the outlet of cooler)	(°C)
P	Pressure	(KPa)
V	Specific volume	(m^3)
n	Polytropic index	-
C_p	Heat capacity at pressure constant	(J/gr.°C)
C_v	Heat capacity at volume constant	(J/gr.°C)

Greek Symbol	**Quantity**	**Unit**
η_{ORC}	Total efficiency of ORC	-
η_{th}	Thermal efficiency of ORC	-
γ	Heat capacity ratio	-
η_E	exergy efficiency of ORC	-
Ω_{ORC}	exergy destruction rate of ORC	-

Subscript	**Quantity**
H.E	shell and tube heat exchanger
Ex	expander
Net	Net
W.F	Working Fluid
E	exergy
th	Thermal
I	Irreversibility
vap	Vaporization
b.p	Boiling Point temperature
M.W	Molecular Weight
C	Critical
I.L	Ideal Liquid
ODP	Ozone Depletion Potential
GWP	Global Warming Potential
PR	Peng-Robinsone

CHAPTER 1

INTRODUCTION

1.1. Background

In recent years, using non-renewable energy source especially fossil fuels as a heat source has caused a number of environmental problems, such as climate change, acid rain, air pollution, and global warming especially with the increasing global demand for many kinds of energy. In this critical situation, attempts are being made to use alternative heat sources instead of fossil fuels as it is one significant way of addressing the environmental issues, but for some processes it is still necessary to use fossil fuel as an energy or heat source. The low and medium temperature range of most commonly available energy resources is between 100 and 200 $^{\circ}$C (Madhawa et al., 2007). Furthermore, the temperature range of industrial waste heat source is typically between ambient temperature and 250 $^{\circ}$C. However, these low and moderate temperature heat sources can hardly be used to generate power through the conventional power generation method (Chan et al., 2013).

Nowadays, the oil price is still high although there has been a significant decrease in 2014. Relatively high oil prices are an obstacle to the development of the global economy especially in countries such as China, India and Iran. On the other hand, various governments have tried to utilize the greenhouse gases such as fluegas produced from boilers to increase the efficiency of fuels and decrease the negative aspects of these kinds of gases such as global warming and also air pollution. As the grade of temperature of this type of gas is slightly higher, therefore it can be used in some thermodynamic effective cycles (Qiu, 2012; Wei et al., 2007; Quoilin et al., 2010). Toward this end, it is proposed that various thermodynamic cycles be considered. These include the Organic Rankine Cycle, Supercritical Rankine Cycle, Kalina Cycle, Goswami Cycle, Trilateral Flash Cycle, and Transcritical Rankine Cycle, which are driven by a number of refrigerant working fluids and they simulate and carry out the conversion of low-grade heat sources into electricity (DiPippo, 2004). The most well-known examples of these effective thermodynamic cycles are: TRC (Transcritical Rankine Cycle), Kalina cycle, and ORC (Organic Rankine Cycle), which have been proposed to convert low temperature thermal energy into power (Chen et al., 2010).

1.2. Effective Thermodynamic Cycles

1.2.1. Kalina Thermodynamic Cycle

The Kalina cycle as shown in Figure 1.1 is more complex and its efficiency is approximately three percent greater than ORC and TRC thermodynamic cycles at simulated and actual analyses, and this is an advantage of this cycle, but the main disadvantage of Kalina cycle is its need for more frequent and more expensive maintenance. Also, the foremost disadvantage of the Kalina cycle compared to ORC is its greater complexity (DiPippo, 2004). Nevertheless, for pure working fluids, during the isothermal evaporation process, the constant evaporation temperature is mismatched with the temperature change of the heat source in the heat exchangers, and this causes a large number of Irreversibilities (Vélez et al., 2011; DiPippo, 2004).

With reference to Figure 1.1, the working solution of ammonia-water mixture entering the turbine (stream 1) is expanded. Energy is recovered from stream 2 to preheat the working solution in recuperator-1. In order to have a low condensation pressure in condenser-1, a separator is used from which a rich ammonia vapour (stream 11) and a lean ammonia liquid (stream 12) are obtained. The lean liquid is mixed with the working solution (in mixer-1) and thus the ammonia mass fraction in condenser-1 is reduced. The mass flow rate in the separator loop is determined by the satisfaction of the pinch point criterion for recuperator-2. A throttle valve is used to bring the pressure of the lean liquid (stream 12) down to the pressure level of the working fluid (stream 4) before mixing in mixer-1. The rich vapor (stream 11) is mixed with the basic solution (stream 8) to again form the working fluid (stream 14) before going through condenser-2 and pump-2 to increase the pressure equal to the turbine inlet pressure. After pump-2, the working fluid is heated up to the turbine inlet temperature in the receiver (Modi & Haglind, 2014).

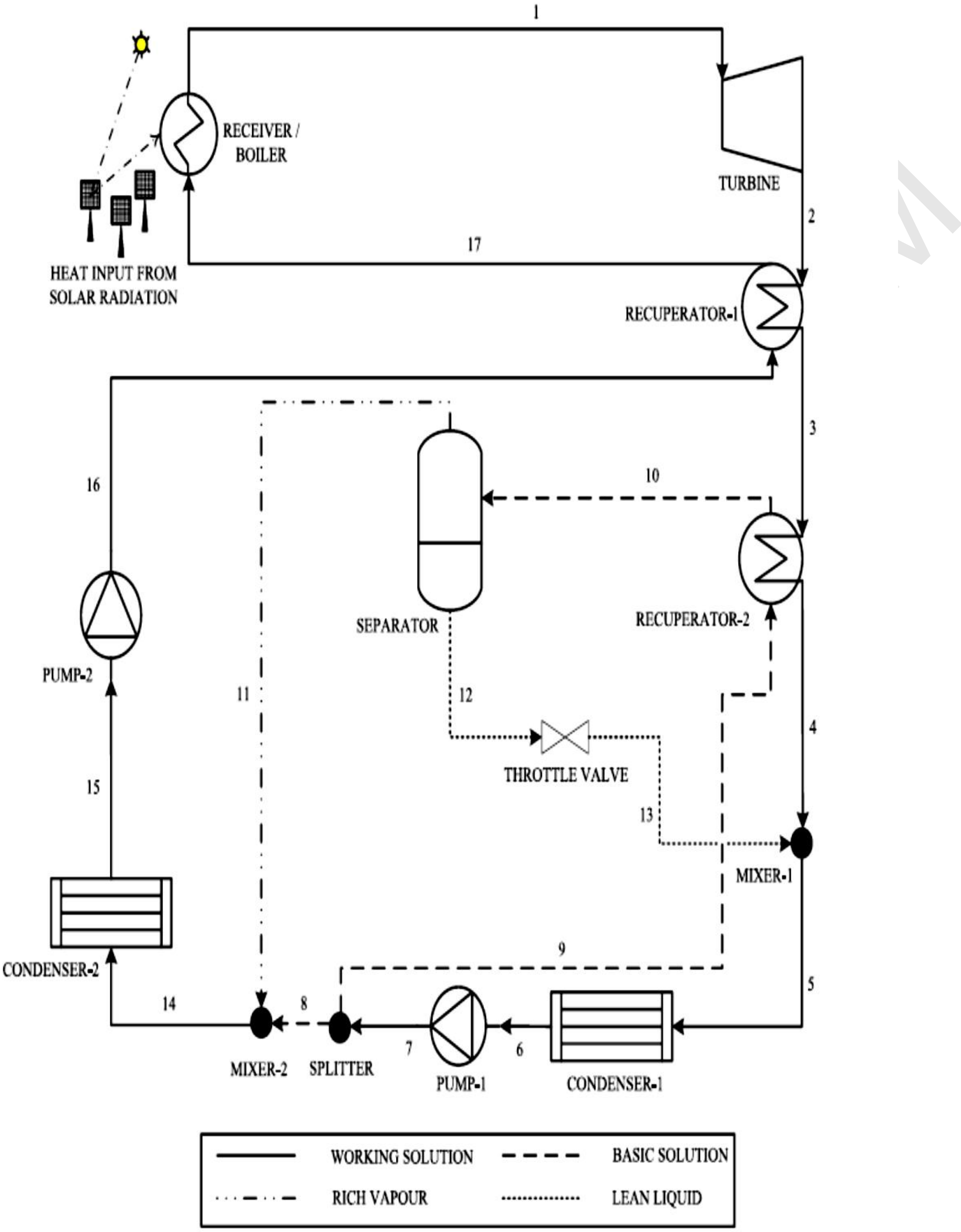
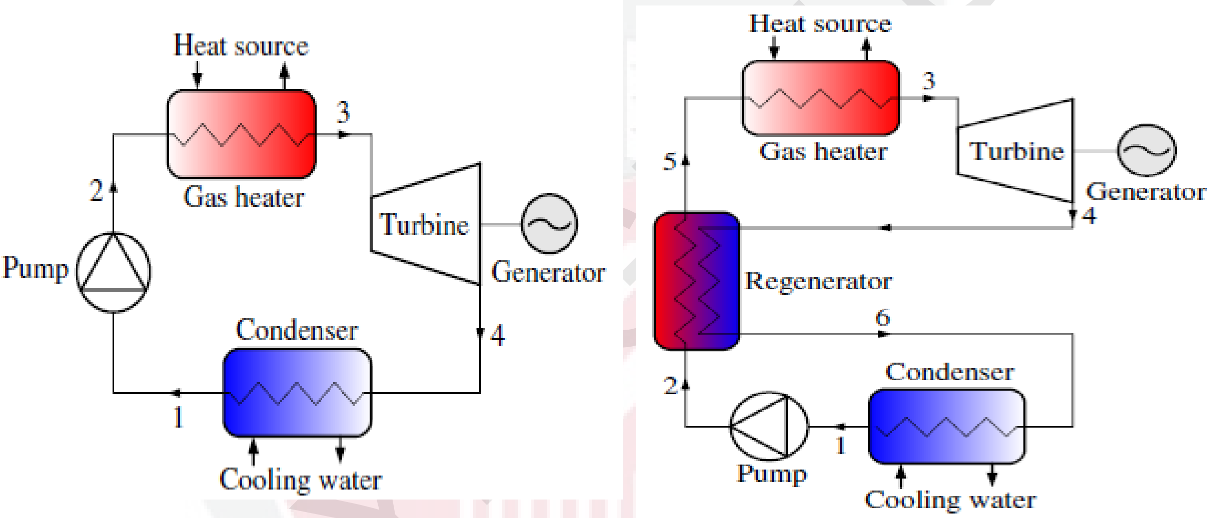


Figure 1.1 Schematic of a Kalina cycle (Modi & Haglind, 2014)

1.2.2. TRC Thermodynamic Cycle

A Transcritical Rankine Cycle (TRC) is a thermodynamic cycle where the working fluid goes through both subcritical and supercritical states. This is often the case when carbon dioxide, CO_2, is mixed by a refrigerant working fluid. However, in the TRC thermodynamic cycle, the working fluid can be heated directly from liquid to the supercritical state, which results in a better thermal match in the gas heater, evaporator, and heat exchanger exactly similar to the ORC thermodynamic cycle, and reduces the energy destruction in the heating process (Karellas & Schuster, 2008). A number of researchers have claimed that the TRC thermodynamic cycle, which is one of those shown in Figure 1.2 (a & b), is similar to the ORC thermodynamic cycle that can be used for low grade heat source and also is more effective in generating electrical energy, which is the main and important purpose of these cycles (Zhang et al., 2006; Cayer et al., 2009).



(a) Without a regenerator **(b) With a regenerator**

Figure 1.2 Schematic of a TRC (Dai et al., 2013)

The CO_2 is an undertaking working fluid for Transcritical Rankine cycles (TRCs) because of some advantages: it is an environmentally-friendly natural working fluid with zero ODP (ozone depletion potential) and a negligible GWP (global warming potential); and it is nonflammable and non-toxic (Cayer et al., 2009). Also it has favorable thermodynamics and transport properties. However, unfortunately, this practical working fluid has a number of disadvantages, some of which are discussed below for improvement. The first and foremost disadvantage of CO_2 is it has a critical point, which is as low as 31.1 $^{\circ}$C and its potential effect on the condensation process due to the temperature limitations of available cooling sources (Chen et al., 2010). Another negative point of CO_2 as a working fluid for TRCs cycles is its high critical pressure, which is as high as 7.38 MPa. The normal operating pressure of a CO_2 system is usually above 10 MPa, which leads to safety concerns in a real and normal operation. On the other hand, instead of CO_2, other working fluids can be used for TRCs cycles such as HFCs (hydrofluorocarbons) and HCs (hydrocarbons) (Gu & Sato, 2002; Saleh et al., 2007; Schuster et al., 2010).

A schematic of the TRC analyzed in this study is shown in Figure 1.2 (a) and Figure 1.2 (b). The difference between these figures is that a regenerator, which acts as an internal heat exchanger to increase the performance of the TRC, is used in the cycle in Figure 1.2 (b). The cycle in Figure 1.2 (b) includes a pump, a gas heater, a turbine, a generator, a condenser, and a regenerator. The working fluid first flows into the pump (point 1), then after being pressurized above the critical pressure (point 2), it flows into the regenerator, where it absorbs heat from the fluid coming from the outlet of the turbine. Next, it goes into the gas heater (point 5) and is heated by the heat source. The supercritical fluid enters the turbine (point 3) and expands to drive a generator to generate power. After expansion, the low-pressure vapor enters the regenerator (point 4) to reject heat to the pressurized fluid from the pump. After decreasing its temperature in the regenerator (point 6), the working fluid flows into the condenser and is condensed to the liquid state. Finally, the fluid returns to the pump (point 1) and completes one cycle (Dai et al., 2013).

1.2.3. ORC Thermodynamic Cycle

The ORC thermodynamic cycle is capable of converting low-grade waste heat source to power. The focus of recent researches has been on solar energy, biomass energy, geothermal resources, power plant waste heat, and fluegas of boilers (Yamamoto et al., 2001; Dai et al., 2009; Wei et al., 2007; Desai et al., 2009). The lower and medium temperatures of heat source of ORC (below 300 $^{\circ}$C) can cause higher thermal efficiencies, reliability and flexibility as well as simpler control and lower maintenance costs for greater economy and effectiveness (Ammar et al., 2012; Aneke & Agnew, 2011; Stoppato, 2012; Roy et al., 2011; Quoilin et al., 2011).

The Organic Rankine Cycle (ORC) applies the principle of the Steam Rankine Cycle, but uses organic working fluids with low boiling points to recover heat from lower temperature heat sources instead of water as a working fluid. Figure 1.3-1.7, shows a configuration of some ORC thermodynamic cycles (Chen et al., 2010; Modi & Haglind, 2014; Sun & Li, 2011; Kang, 2012; Wang et al., 2013). ORC thermodynamic cycle has a number of advantages such as; its simple structure, the availability of its components, the ease of application for local small-scale power generation systems, and driven by low-grade heat sources with temperature lower than 370 $^{\circ}$C and below this temperature called low-grade temperature in industry. The structure of ORC thermodynamic cycles is similar to a typical Rankine Cycle (RC) which uses water as a working fluid, but in ORC systems the organic fluids especially refrigerant fluids are used as working fluids with high critical coordinate values, because of lower specific vaporization (Wang et al., 2011; Yamamoto et al., 2001; Kang, 2009; Dai et al., 2009; Wei et al., 2007).

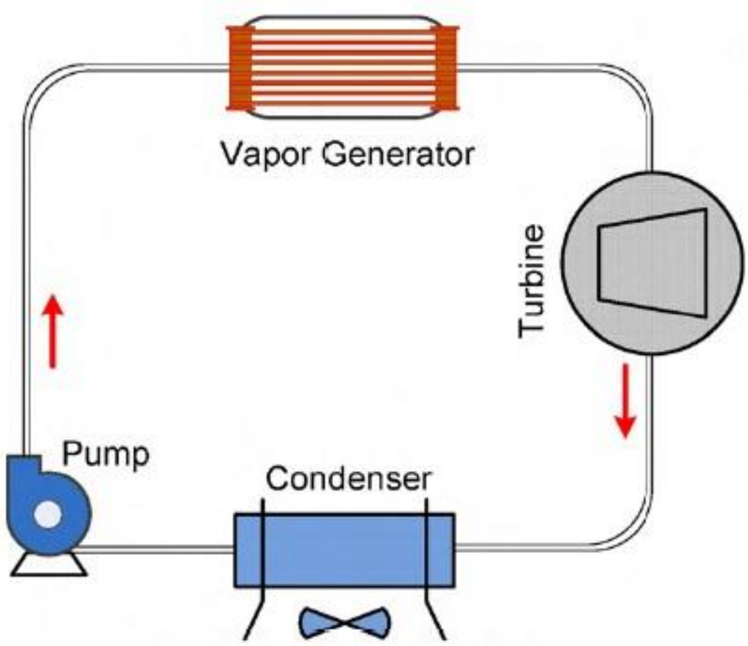


Figure 1.3 Schematic of a ORC (Chen et al., 2010)

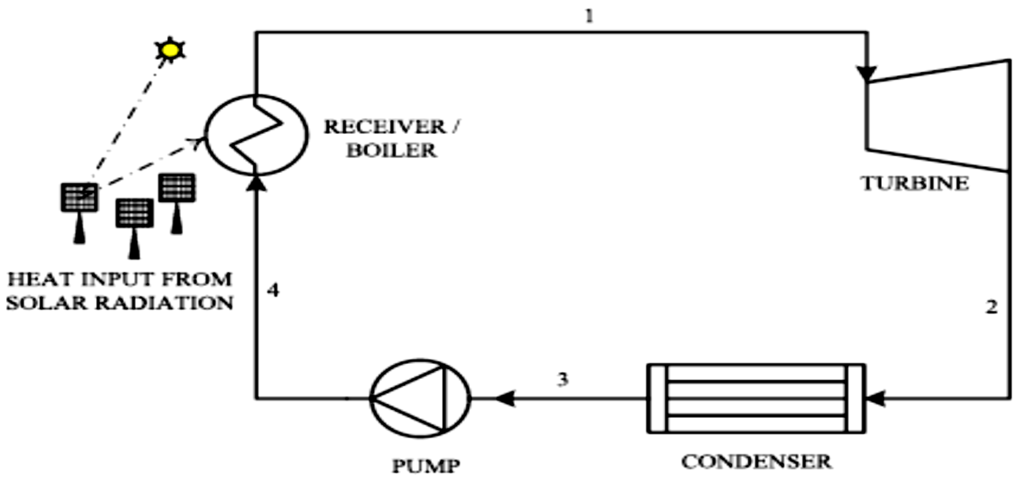


Figure 1.4 Schematic of a ORC (Modi & Haglind, 2014)

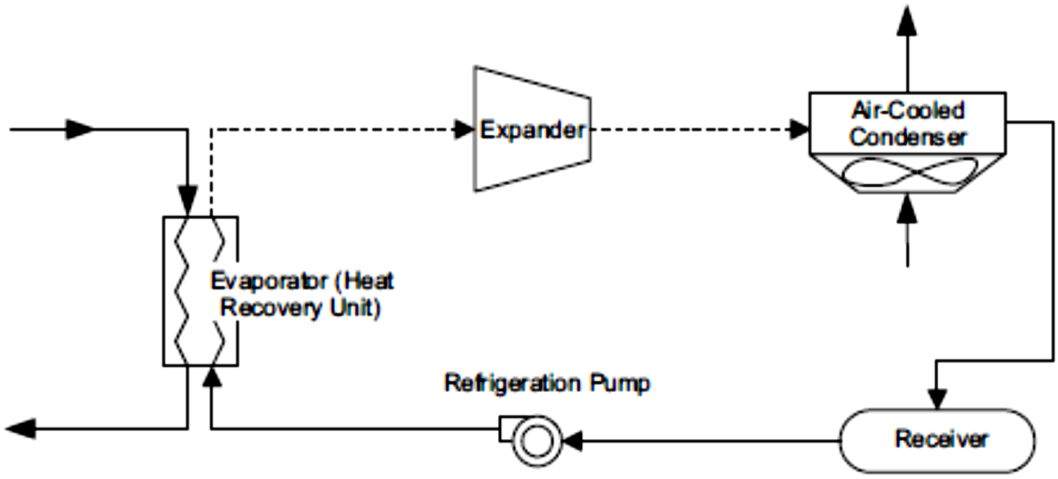


Figure 1.5 Schematic of a ORC (Sun & Li, 2011)

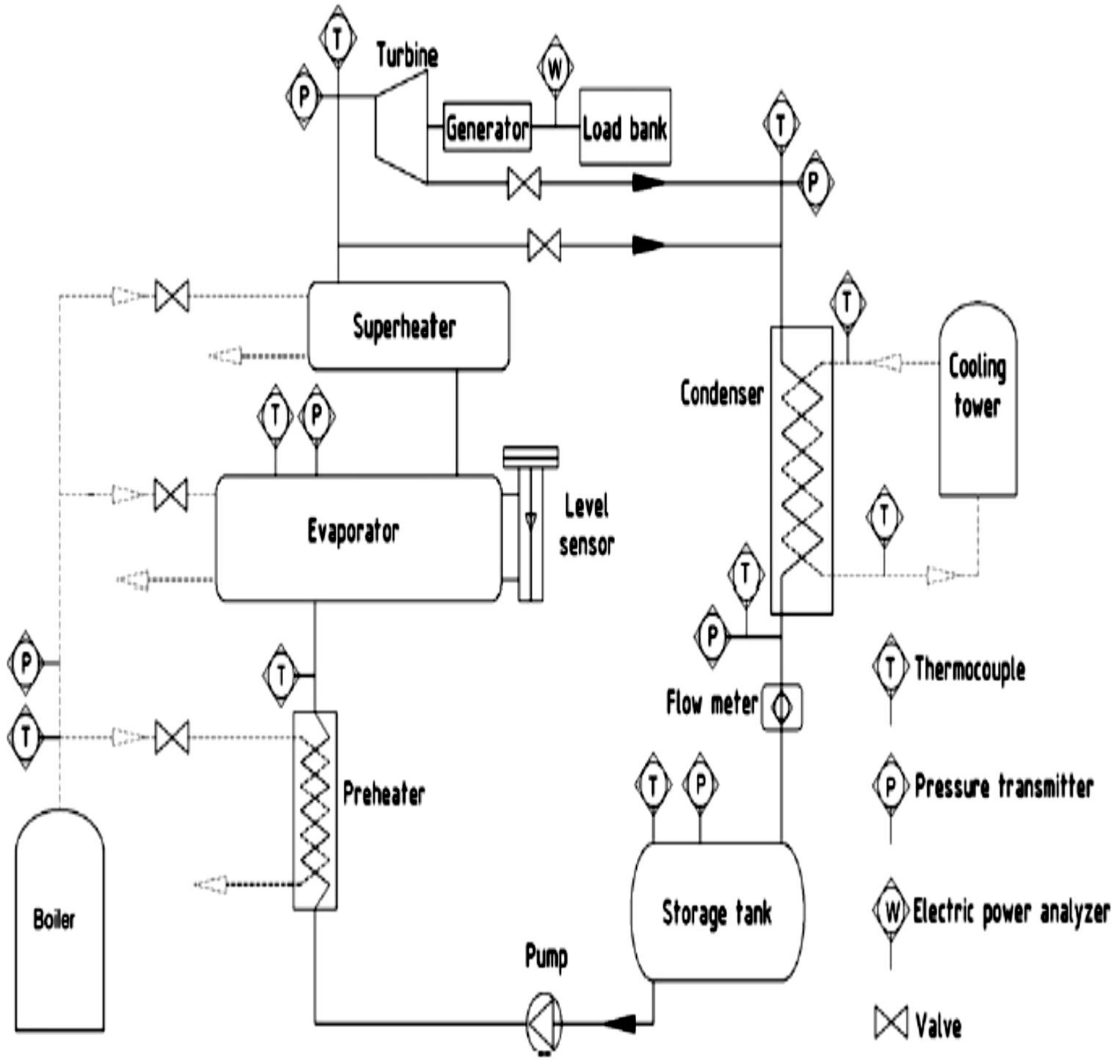


Figure 1.6 Schematic of a ORC (Kang, 2012)

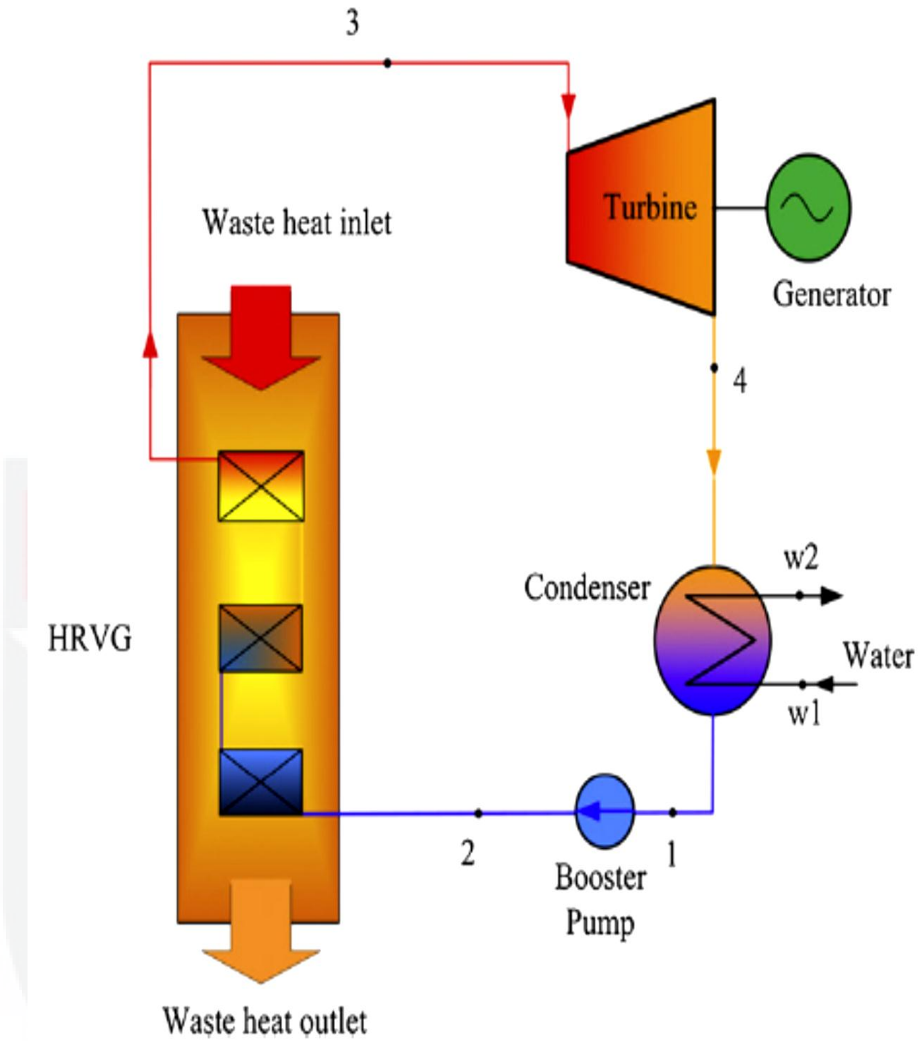


Figure 1.7 Schematic of a ORC (Wang et al., 2013)

1.3. Refrigerant Working Fluids

Pure working fluids especially wet, isentropic, and dry fluids including:

- Chlorofluorocarbons (CFCs) (Yari, 2010; Lakew & Bolland, 2010; Guo et al., 2011).
- Hydrofluorocarbons (HFCs) (Tchanche et al., 2009; Saleh et al., 2007; Yari, 2010; Lakew & Bolland, 2010; Guo et al., 2011; Tempesti et al., 2012).

- Hydrocarbons (HCs) (Tchanche et al., 2009; Saleh et al., 2007; Lakew & Bolland, 2010; Guo et al., 2011; Aljundi, 2011; Liu & Duan, 2012).

- Hydrocholoroflurocarbons (HCFCs) (Zhang et al., 2011; Chen et al., 2010; Gua et al., 2011; Mikielewicz & Mikielewicz, 2010; Wang et al., 2012;

Maizza & Maizza ,1996; Kosmadakis et al., 2009; Dai et al., 2009; Li et al., 2012; Li et al., 2011).

- Hydrofluroethers (HFEs) (Wang et al., 2011; Tokuhashi et al., 2000; Murata et al., 2002; Yasumoto et al., 2003; Defibaugh et al., 1192; Wang et al., 1991).

These refrigerant working fluids are generally selected as the working fluids for ORC thermodynamic cycles and in terms of relation of Entropy differences and Temperature differences at operating conditions are classified as wet, isentropic, or dry fluids. An ideal ORC should have a perfect match between the temperatures of the working fluid and the heat source to reduce exergy losses during the heat transfer. Subcritical ORCs, which are operated at pressures below the critical point, have isothermal evaporation and condensation processes that result in worse temperature matches between the working fluid and the heat source, which lead to large heat transfer Irreversibilities (Shiflett & Yokozeki, 2007; Chen et al., 2012). In contrast, supercritical ORCs can have better temperature matches with the heat source; however, their operating pressures are much higher than for the subcritical cycles. The heat exchangers in supercritical ORC thermodynamic cycles are also larger since the overall heat transfer coefficient decreases as the operating pressure increases (Chen et al., 2011).

This study first attempts to investigate R245fa from HFC refrigerant fluids group; secondly investigates NOVEC 7000 from HFE refrigerant fluids group, and thirdly, R141b is considered from HCFCs group as refrigerant working fluids, because of high heat of vaporization ($\Delta h_{vap.}$) and high density in vapor state ($\rho_{vap.}$), compared with other refrigerant fluids. An ORC thermodynamic cycle is then designed and simulated by using these refrigerant working fluids and driven by fluegas to generate optimum power i.e. more than 3MW that proper amount of energy for applying in refinery and petrochemical industries, such as; NGL 1300 factory of Khozestan, Iran and NGL 1200 factory of Fars, Iran (Amini et al., 2012). The wet fluegas, which is used in this ORC thermodynamic cycle is combustion and burn from natural gas and drive by air ambient (Beychok, 2012).

1.4. Research Problem Definition

A large group of researchers (Pei et al., 2011; Wei et al., 2007; Yamamoto et al., 2001; Roy & Ashok, 2012; Heberle et al., 2012) have focused on achieving the total efficiency of ORC below 50 %, however this study try to modify and increase total efficiency of ORC higher than 50 %, also improve total exergy efficiency and power generator efficiency, means polytropic efficiency, and decrease the exergy destruction rate to generate optimum power.

By applying simple and economic operating condition like: normal, steady state, and subcooled liquid instead of complex operating conditions like supercritical, superheating and so on (Chen et al., 2012; Roy & Misra, 2012), try to improve and increase the power generation in optimum by using ORC.

Another obstacle goes back to the waste gases of equipment at refineries and petrochemical plants especially fluegas of boilers. These waste gases have a high temperature (>150 $^{\circ}$C) and also have harmful environmental compounds such as: CO_2, N_2, O_2, and H_2O which cause a number of environmental problems, such as global warming, climate change, acid rain, and air pollution. Therefore, the current study tries to use wet fluegas of boilers combustion and burn from natural gas to avoid removing the fluegas from Boilers to the environment with high temperature and also high amount of compounds. And as a result, with increasing the heat transfer from fluegas to working fluids attempts to improve and increase the total efficiency of ORC and in same line improve and increase the polytropic efficiency of expander as power generator efficiency.

Finally, the last advantage of this study is using the HYSYS simulation software to decrease operational costs in industry at real level, and also decrease the number of errors at implementation of each section of the current study and increase the safety of this study by using this powerful Chemical Engineering simulation software.

1.5. Objectives of Study

The main objectives of this study are:

i) To investigate and simulate the ORC thermodynamic cycle of this study by using R245fa, NOVEC7000, and R141b as working fluids and driven by fluegas and using HYSYS.
ii) Evaluate the optimum power generated by expander from the ORC thermodynamic cycle between R245fa, NOVEC 7000, and R141b as working fluids and driven by fluegas and using HYSYS simulation.

1.6. Scope and Relevance of Study

Nowadays, optimum power is being generated by using a simple and low maintenance thermodynamic cycle and applying waste gases with high temperature and harmful compounds that have more environmental issues for industries especially at refineries and petrochemicals. Hence, using the model of current ORC by HYSYS simulation software in this study will try to generate optimum power through wet fluegas combustion and burn from natural gas and drive by air ambient that including 70 % Nitrogen (N_2), 9 % Carbon Dioxide (CO_2), 2 % Oxygen (O_2), and the rest others belong to water (H_2O) approximately 19-20 % (Beychok, 2012). The high temperature of fluegas of boilers as a heat source of heat exchanger applied to change phase fraction of working fluids from 0 to 1. Current ORC is a simple idealized thermodynamic cycles because including isentropic process at pump and expander and isochoric process at heat exchanger and cooler. This ORC is driven by three well-known refrigerant working fluids with normal, steady state, and subcooled liquid as initial operating condition. For simulation the present ORC and generating optimum power the following steps should be observe:

1.6.1. Define Working Fluids and fluegas for HYSYS

First of all in a simulation of the current ORC by HYSYS there is a need to define R245fa from HFC group, NOVEC7000 from HFE group, and R141b from HCFCs group as refrigerant working fluids. Because HYSYS has a limited library source with a number of specific materials but does not including these working fluids. In order to describe each working fluid there should be input of some thermodynamic parameters which consist of: component name (working fluid name), UNIFAC structure (molecular structure), molecular weight ($m_{M.W}$), boiling point temperature at normal thermodynamic condition ($T_{b,p}$), ideal liquid density ($\rho_{I.L}$), critical temperature (T_c), critical pressure (P_c), and critical volume (V_c). But to define fluegas for HYSYS the components of fluegas: H_2O, CO_2, N_2 and O_2 should be found and input from the library of HYSYS then added to the component list along working fluid.

1.6.2. Selecting a Suitable Fluid Package as a Solvent Method

The last step to prepare the HYSYS for starting the simulation of the present ORC system is selecting a suitable fluid package as a solvent method for estimate and solve a lot of parameters (such as thermodynamic and heat parameters) by HYSYS which are needed for simulation and analysis of the present ORC system. The main function of each fluid package is similar, but the differences are in accuracy of the calculations. The current study selects and uses Peng-Robinson (PR) fluid package as a solvent method of ORC simulation, because it has the highest accuracy compared with other fluid packages such as: steam package, CS, GS, Activity models, and PRSV.

1.6.3. Define, Add, and Simulate each Instrument of the Present ORC to Simulate the Whole Present ORC

Now the preparation of HYSYS to start the simulation of the present ORC system is completed. It is now time to add the fluids flow of each working fluid and instruments of ORC and also simulate in PFD-case of HYSYS (simulation environment of HYSYS). Here the important objective is to define the subcooled, normal, and steady state of the initial operating condition for first fluid flow of each working fluid. Another more important objective in simulation of each fluids flow and also each instrument of ORC selects the suitable thermodynamic and heat parameters at input and output of each fluids flow and instruments of ORC for decreasing error to least, because of safety and also high efficiency at each section.

1.6.4. Energy Analysis of ORC

By using Energy analysis of ORC such as: Grid diagram of ORC, Grid diagram of heat exchangers, heat exchangers detailed characteristics and capital cost index, T-H diagram of heat exchangers, and tables of Grid Diagrams data of heat exchangers, can encourage deeper thinking to consider more thermodynamic and heat parameters.

1.6.5. The Theoretical Formulas of ORC

By focusing intensely on some theoretical formula of ORC such as: the maximal net power output of ORC ($\dot{W}_{net}$), heat transfer between fluegas to working fluid ($\dot{Q}_{H.E}$), expander size (SP), total heat transfer capacity (UA_{total}), Irreversibility and exergy (I & E), total efficiency of ORC (η_{ORC}), thermal efficiency of ORC (η_{th}), polytropic efficiency of expander, exergy efficiency of ORC, and exergy destruction of ORC, and by paying attention to some thermodynamic and heat parameters that are calculated by simulation, can lead to more investigation and philosophical thinking in this study.

1.7. Hypothesis

The hypotheses of the present study are:

- Increasing the mass flow rate of each refrigerant working fluid leads to increasing the electricity generated by expander.
- Increasing the net power output of expander and total exergy of ORC increases the maximal net power output of ORC.
- Increasing the value of heat transfer between fluegas to each working fluid leads to improve and increase the efficiency of ORC.
- Gliding inlet pressure of expander increases inlet temperature of expander then net power of expander is increased.
- The thermal efficiency of ORC should be always smaller than the total efficiency of ORC.

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