ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE ENGINEERING AND TECHNOLOGY

WORKING FLUID RANKING USING COSMO AND REFPROP SOFTWARES FOR A MOBILE WASTE HEAT RECOVERY SYSTEM

M.Sc. THESIS

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Department of Mechanical Engineering

Automotive Engineering Programme

OCTOBER 2017

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ISTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

BİR SEYYAR ATIK ISI GERİ KAZANIM SİSTEMİ İÇİN COSMO VE REFPROP PROGRAMLARI KULLANILARAK AKIŞKANLARIN SIRALANMASI

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To my father,

FOREWORD

I studied waste heat recovery systems during my professional career at Ford Otosan. I thought that I could make a significant contribution in the literature by writing my Master of Science thesis in this field. I believe that the conclusion of this thesis can be used in the automotive industry to improve fuel economy.

I would like to thank my supervisor Emre Özgül for his support. I would like to thank also Serdar Güryuva for his support and guidance.

October 2017

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ABBREVIATIONS

WHR	**:** Waste Heat Recovery
FE	**:** Fuel Economy
AIGK	**:** Atık Isı Geri Kazanım Sistemi
OEM	**:** Original Equipment Manufacturer
ORC	**:** Organic Rankine Cycle
CAMD	**:** Computer Aided Molecular Design
1D	**:** One Dimensional

SYMBOLS

p_evap_out	: Evaporation pressure at next time step
T_cond_actual	: Actual condensation temperature
p_cond_target	: Target condensation pressure
subcool	: Condenser outlet subcool
superheat	: Evaporator outlet superheat
h2	: Enthalpy at pump outlet
tailpipe_temp	: Tailpipe temperature, gas temperature at evaporator inlet
p_ambient	: Ambient pressure
p_cond_actual	: Actual condensation pressure
p_evap_in	: Evaporation pressure at current time step
h23b	: Enthalpy of working fluid at evaporator where it is fully evaporated
T_evap	: Evaporation temperature
h1	: Enthalpy of working fluid at pump inlet
h2s	: Isentropic enthalpy at pump outlet
h23a	: Enthalpy of working fluid at evaporator where it begins to evaporate
h3	: Enthalpy of working fluid at expander inlet
h4s	: Isentropic enthalpy at expander outlet
T2	: Temperature of working fluid at pump outlet
T_cond_target	: Target condensation temperature
h41a	: Enthalpy of working fluid at condenser where it begins to condense
s3	: Entropy of working fluid at expander inlet
pp_cond	: Pinch point temperature difference at condenser
cp_coolant	: Coolant specific heat
T_coolant_in_actual	: Actual coolant temperature at condenser inlet
wf_pump_eff	: Efficiency of working fluid pump
exp_eff	: Expander efficiency
pp_evap	: Pinch point temperature difference at evaporator
h_exh_in	: Exhaust gas enthalpy at evaporator inlet
h_exh_out	: Exhaust gas enthalpy at evaporator outlet
cp_exh	: Specific heat of exhaust gas
T_exh_out	: Exhaust gas temperature at evaporator outlet
T_exh_in	: Exhaust gas temperature at evaporator inlet
air_flow	: Airflow rate of internal combustion engine
fuel_flow	: Fuel flow rate of internal combustion engine
s1	: Isentropic enthalpy at pump inlet
m_coolant_target	: Target coolant mass flow rate
T_coolant_in_target	: Target coolant temperature at condenser inlet
P_exp	: Power generated by expander
P_wf_pump	: Power consumed by working fluid pump

q_cond : Condenser heat rejection
dT2 : Pinch point temperature difference at evaporator inlet
dT23a : Pinch point temperature difference at evaporator where working fluid begins to evaporate
dT23b : Pinch point temperature difference at evaporator where working fluid is fully evaporated
dT3 : Pinch point temperature difference at evaporator outlet
T_exh_out_next : Exhaust gas temperature at evaporator outlet at next time step
m_wf : Working fluid mass flow rate
q_evap : Heat transfer rate through evaporator
m_exh : Mass flow rate of exhaust gas
h4 : Enthalpy of working fluid at expander outlet
T3 : Working fluid temperature at expander inlet
T_exh_23a : Exhaust gas temperature at evaporator where working fluid begins to evaporate
T_exh_23b : Exhaust gas temperature at evaporator where working fluid is fully evaporated
dTmin : Minimum of pinch point differences
T_41a_coolant_target: Target coolant temperature at condenser section where working fluid begins to condense
P_net : Net power generated by waste heat recovery system
FE_Benefit : Fuel economy benefit of the waste heat recovery system
Q_wf : Volume flow rate of working fluid

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WORKING FLUID RANKING USING COSMO AND REFPROP SOFTWARES FOR A MOBILE WASTE HEAT RECOVERY SYSTEM

SUMMARY

A simulation methodology is developed for the working fluid assessment using COSMO and REFPROP softwares for a WHR system that employs Rankine cycle to generate useful work by utilizing waste exhaust heat of a heavy-duty internal combustion engine. The methodology has two distinct approaches for working fluid assessment compared to the methodologies in literature. First, it compares the working fluids in transient cycles rather than at a limited number of steady state operating points. Secondly, a fixed condensation pressure is used as a constraint rather than fixed condensation temperature. These two approaches enable a more realistic working fluid assessment.

Two fluid properties are developed with COSMO and REFPROP softwares. These fluid properties models are interchangeable without any need to modify the main integrated model. A Rankine cycle model is developed in Simulink to carry out thermodynamic calculations. A cooling model is also developed in GT-SUITE in order to factor in the effect of pump and fan power consumption. These three models are integrated in Simulink model. A Matlab script is written for each fluid properties model to run the integrated model iteratively for different working fluids.

Simulations are carried out for 146 working fluids that are commonly analyzed in literature. Simulation results show that ethenol provides the highest fuel economy benefit when working fluid properties are calculated with COSMO software whereas cyclopentane provides the highest fuel economy benefit when working fluid properties are calculated with REFPROP. Moreover, COSMO fuel economy results are compared to REFPROP fuel economy results and it is shown that COSMO results are in good agreement with REFPROP results. However, the use of predictive softwares such as COSMO affects the working fluid ranking. Hence, an empirical software or data should be used for fluid properties for a precise working fluid ranking. As a result, it is concluded that cyclopentane is the most suitable working fluid to be used in a WHR system for a heavy-duty engine for the best fuel economy and environmental safety.

BİR SEYYAR ATIK ISI GERİ KAZANIM SİSTEMİ İÇİN COSMO VE REFPROP PROGRAMLARI KULLANILARAK AKIŞKANLARIN SIRALANMASI

ÖZET

İnsan sağlığını tehlikeye atan en önemli faktörlerden birisi solunum yoluyla alınan havadaki zehirli gazlardır. Havadaki zehirli gazların en büyük kaynağı araçlardan salınan egzoz gazlarıdır. Zararlı egzoz gazlarının salınımını ve yakıt tüketimini azaltmak için devletler tarafından konulan regülsayonlar her geçen yıl daha da zorlayıcı olmaktadır. Araç üreticileri bu regülasyonları sağlayabilmek için çok çeşitli teknolojiler üzerinde çalışmaktadır.

Emisyon ve yakıt tüketimini azaltmayı sağlayan teknolojilerden biri de atık ısı geri kazanım (AIGK) sistemleridir. AIGK sistemlerinde Rankine çevrimi ile egzoz gazındaki atık ısı enerjisi geri kazanılarak iş üretilmektedir. AIGK sistemi temel olarak pompa, buharlaştırıcı, genleştirici ve yoğunlaştırıcı parçalarından oluşmaktadır. Bunlara ek olarak yoğunlaştırıcıdan atılan ısıyı dış ortama atmak için su pompası, radyatör ve fandan oluşan bir soğutma sistemi kullanılmaktadır. AIGK sisteminde pompa ile akışkanın sistemde devir daim etmesi sağlanmaktadır. Pompadan çıkan akışkan buharlaştırıcıda egzoz gazı ile buharlaştırılmaktadır. Buharlaştırıcıdan çıkan buhar halindeki ve basınçlı akışkan ile genleştiricide güç üretimektedir. Genleştiriciden çıkan düşük basınçlı buhar halindeki akışkan yoğunlaştırıcıdan geçirilerek sıvı hale geçmektedir. Genleştiriciden çıkan akışkan tekrar pompaya gelerek sistemde devir daim etmektedir. Yoğunlaştırıcıdan soğutma suyuna atılan ısı bir fan yardımıyla radyatörden dış havaya atılmaktadır. Bu sistemde genleştirici güç üretirken AIGK sistemi pompası, su pompası ve soğutma fanı güç tüketmektedir. Üretilen net güç elektrikli veya mekanik yöntemlerle motora aktarılarak emisyonların ve yakıt tüketiminin azaltılması sağlanmaktadır.

AIGK sistemlerinde üretilen net gücü etkileyen birçok faktör vardır. Bunlardan bazıları buharlaştırıcı tasarımı, genleştirici tasarımı, yoğunlaştırıcı tasarımı ve sistemde kullanılan akışkandır. Bu çalışmada sistemde kullanılabilecek farklı akışkanların yakıt tüketimine etkisi incelenmiştir. Bu amaçla Matlab Simulink programında bir model oluşturulmuştur. Bu model üç alt modelden oluşmaktadır. Bunlardan birincisi akışkan özelliklerini hesaplamaktadır. Akışkanların özelliklerini hesaplamak için iki farklı yöntem kullanılmıştır. Birincisi test verilerini temel alan fonksiyonları kullanan REFPROP programıdır. Diğeri ise PubChem veritabanından her akışkan için indirilen molekül yapısını kullanarak termodinamik ve kuantum fiziği hesaplamaları ile akışkan özelliklerini tahmin eden COSMO programıdır. İkinci alt model ise bir Simulink fonksiyonu ile oluşturulan Rankine çevrimi hesaplamalarını yapan modeldir. Bu model AIGK sistemi pompasının basması gereken akışkan debisi, buharlaştırıcı ısı transferi, genleştiricide üretilen güç, yoğunlaştırıcı ısı transferi gibi değerleri hesaplamaktadır. Üçüncü alt model ise tek

boyutlu sistem simülasyon programı olan GT-SUITE programında kurulmuş olan soğutma sistemi modelidir. Soğutma sistemi modelinde AIGK sistemindeki akışkanın yoğunlaşma basıncı hava basıncına eşit olacak şekilde fan hızı ayarlanmakta ve su pompasının çektiği güç, fanın çektiği güç, su sıcaklığı gibi değerler hesaplanmaktadır. Üç alt model birbiriyle birleştirilerek bütünleşmiş bir şekilde çalışması sağlanmıştır. Rankine çevrimi hesaplamalarını yapan modelin çıktıları diğer iki modele beslenmekte ve bu modelleirin çıktıları tekrar Rankine çevrimi modeline beslenmektedir. Yakıt tüketimi iyileşmesini karşılaştırmak için zamana bağlı araç test verisi kullanılmıştır. Bu test verisinden egzoz debisi ve sıcaklığı değerleri alınmıştır. Son olarak, tüm bu hesaplamaları her akışkan için tekrarlatan ve sonuçları kaydeden REFPROP ve COSMO için iki ayrı Matlab kodu yazılmıştır. Her iki yöntem ile akışkanlar yakıt tüketimi iyileşmesine göre sıralanmış ve iki program ile elde edilen sonuçlar karşılaştırılmıştır.

COSMO ve REFPROP ile hesaplanan akışkan özellikleri karşılaştırıldığında sonuçların bazı akışkanların bazı özellikleri için yakın olduğu gözlemlenmiştir. Benzer şekilde sonuçlar bazı akışkanların bazı özellikleri için de çok farklı olabilmektedir.

Zamana bağlı REFPROP simülasyon sonuçlarına bakıldığında bazı akışkanlar için hedef yoğunlaşma basıncı sağlanamamıştır. Bunun nedeni kullanılan fanın yeterli soğutmayı sağlayamamasıdır. Bu nedenle yoğunlaşma basıncı ve sıcaklığı yüksek kalabilmektedir.

REFPROP sonuçlarına bakıldığında bazı akışkanların ısı kapasitelerinin düşük olmasından dolayı buharlaşma sıcaklıklarının düşük olduğu gözlemlenmiştir. Isı kapasitesi düşük olan akışkanlar buharlaştırıcıda sıvı fazda çok hızlı ısınmakta ve sıvı sıcaklığı egzoz sıcaklığına çok hızlı yaklaşmaktadır. Bu nedenle daha erken sıcaklıkta buharlaşmakta ve buharlaşma sıcaklığı düşük olmaktadır.

REFPROP sonuçlarından çıkarılan bir diğer sonuç buharlaşma sıcaklığı ile yakıt tüketimi iyileşmesi arasında doğru orantı olmasıdır. Bu sonuç Rankine çevriminde buharlaştırmanın ne kadar yüksek sıcaklıkta ve yoğulaştırmanın ne kadar düşük sıcaklıkta yapılırsa verimliliğin o kadar yüksek olacağı gerçeği ile uyumludur. Tüm akışkanların yoğunlaşma basıncı ortam basıncına eşit olmasına çalışıldığından dolayı yoğunlaşma sıcaklığı tüm akışkanlar için birbirine yakın değerler almaktadır. Bu nedenle Rankine çevriminin verimliliğini etkileyen tek etken olarak buharlaşma sıcaklığı kalmaktadır. Sonuçlarda da gösterildiği gibi buharlaşma sıcaklığı ne kadar yüksek ise yakıt tüketimi iyileşmesi o kadar yüksek olmaktadır.

Simülasyon sonuçlarına göre akışkan özellikleri COSMO programı ile hesaplandığında en iyi yakıt tüketimini sağlayan akışkanın ethenol olduğu bulunmuştur. Akışkan özellikleri REFPROP programı ile hesaplandığında ise en iyi yakıt tüketimi iyileşmesi sağlayan akışkanın siklopentan (cyclopentane) olduğu bulunmuştur. COSMO sonuçları ile REFPROP sonuçları karşılaştırıldığında en iyi yakıt tüketimi iyileşmesine göre sıralamanın birebir aynı olmasa da birbirine çok yakın olduğu bulunmuştur. Ancak en iyi yakıt tüketimi iyileşmesini sağlayan akışkan her iki program ile birbirinden farklı bulunmuştur.

Molekül yapısına bakarak tahmin yapan COSMO programına göre REFPROP programı test verilerini esas aldığından REFPROP ile elde edilen akışkan sıralamasının daha güvenilir olduğu sonucuna varılmıştır. Dolayısıyla COSMO programı test verisi olmayan veya olan milyonlarca akışkanın değerlendirilmesi için uygun bir program olarak kullanılabilir. Ancak daha kesin ve nihai akışkan değerlendirmeleri için test verisini esas aldığından REFPROP programı kullanılmalıdır. Sonuç olarak bu uygulamada kullanılan sınır koşullarına göre kullanılabilecek olan en iyi akışkanın siklopentan (cyclopentane) olduğu sonucuna varılmıştır.

1. INTRODUCTION

The emission regulations are becoming more and more stringent and customer expectations are increasing. Automotive OEMs are working on several technologies to reduce CO_2 emissions and to imrove fuel economy. Waste heat recovery systems are one of these technologies. Waste exhaust heat is converted to useful work with a Rankine cycle. In this thesis, several working fluids were analyzed for the best fuel economy benefit.

1.1 Purpose of Thesis

The purpose of this work is to find the ideal working fluid for a waste heat recovery (WHR) system for a long haul truck. The WHR system will be based on subcritical Rankine cycle. The ideal working fluid should have a high fuel economy benefit and should be safe to environment and humans. A new methodology is developed for the calculation of fuel economy benefit of working fluids for a WHR system.

1.2 Literature Review

In literature, there is a lot of research on working fluid assessments for WHR systems.

Schwöbel et al. (2016) analyzed more than 72 million fluids from PubChem database by using commercial COSMO software and concluded that the top three best performing fluids are acetaldehyde, 1,2-difluoroethane (R-152), and methyl formate (R-611) [1].

Frutiger et al. (2016) analyzed 1965 working fluid candidates for an ORC using a low temperature heat source. Peng-Robinson equation of state is used to calculate working fluid properties and it is concluded that octafluorocyclobutane (RC318) is the best performing working fluid [2].

Stijepovic et al. (2016) followed a systematic approach toward the design of Organic Rankine Cycles (ORC) for the generation of power from multiple heat sources available at different temperature levels. It is found out that the optimum solution consists of a system with two Rankine cycle cascades which operate using Benzene and 1,1,1,3,3-Pentafluoropropane as working fluids [3].

Cignitti et al. (2017) found out that 2,2,3,3,4,4,5,5-octa fluorohexane is the optimal working fluid for waste heat recovery of the exhaust gas from a marine diesel engine [4].

Wang et al. (2017) carried out an analysis of organic Rankine cycle (ORC) using hydrofluoroethers as working fluids under constant external conditions and found out that HFE7000 can be used as working fluid in ORC to convert low-grade heat into power [5].

Li et al. (2015) suggested using R245fa for low temperature heat sources and R601a for the high temperature heat sources [6].

There are several studies [7-13] in literature that use computer-aided molecular design (CAMD) which results in virtual fluids. In order to calculate working fluid properties, molecular based equations of state like BACKONE [14] or PC-SAFT [15]. However, in order to use these methods, some parameters from experimental data should be known. Instead of these methods, COSMO software is used which enables to calculate working fluid properties with a completely predictive methodology independent of experimental data.

1.3 Hypothesis

In most of literature studies, working fluids are analyzed at a limited number of steady state vehicle operating points. Moreover, working fluids are compared with the fixed condensation temperature constraint in order to cancel out the effect of cooling system and accessory load of coolant pump and cooling fan. Nevertheless, it is possible to end up with unrealistic working fluid ranking with this approach.

First, vehicle usage is transient most of the time in nature and it is very hard to select representative steady state vehicle operating points.

Secondly, when using fixed condensation temperature, condensation pressure will be either higher or lower than ambient pressure for every working fluid. When condensation pressure is lower than ambient pressure, it will be necessary to limit the condensation pressure to prevent air leakage from ambient to WHR system. When condensation pressure is higher than ambient pressure, there is a possibility of underestimating the fuel economy benefit of the working fluid, because it may have higher fuel economy benefit at a lower condensation pressure. Hence, in order to have realistic results, working fluids should be compared with fixed condensation pressure rather than fixed condesation temperature. In order to be able to carry out simulations with fixed condensation pressure, cooling system should be taken into account to factor in the cooling accessory losses due to different condensation temperatures.

2. SIMULATION METHODOLOGY

The simulation methodology for working fluid ranking is described in the following sections. Two fluid properties models are developed to calculate working fluid properties with COSMO and REFPROP software packages. A function in Simulink is written to carry out Rankine cycle calculations. A 1D cooling model in GT-SUITE is built to carry out cooling calculations. These models are integrated in Simulink and two *.m files for COSMO and REFPROP are written to run the integrated Simulink model for working fluid iterations. The simulations are carried out in a transient vehicle cycle.

2.1 Fluid Properties Model

Working fluid properties are needed to carry out Rankine cycle simulations. Working fluid properties can be calculated by either predictive methods such as COSMO software or empirical methods such as REFPROP software. In this study, both of these software packages are used to calculate working fluid properties and the fuel economy results are compared.

Both fluid properties models are the same in terms of inputs and outputs and they are interchangeable without any change in the integrated model.

The inputs of the fluid properties models are p_evap_out, T_cond_actual, p_cond_target, subcool, superheat, h2, tailpipe_temp, p_ambient.

The outputs of the fluid properties models are p_cond_actual, p_evap_in, h23b, T_evap, h1, h2s, h23a, h3, h4s, T2, T_cond_target, h41a.

Actual condensation temperature (T_cond_actual) is used to calculate actual condensation pressure (p_cond_actual) by looking up from saturation curve.

In order to calculate p_evap_in, evaporation pressure is calculated at (tailpipe_temp-superheat) temperature. This evaporation pressure is limited by maximum 40-bar pressure in order to avoid very high evaporation pressures that will require high cost evaporator with high durability. It is also limited by a 0.8 factor of corresponding critical pressure to ensure stability by staying away from critical state.

Enthalpy of fully evaporated working fluid (h23b) is calculated by looking up from saturation vapor curve at corresponding evaporation pressure.

Evaporation temperature of working fluid (T_evap) is calculated by looking up from saturation vapor curve at evaporation pressure.

Enthalpy of working fluid at pump inlet (h1) is calculated by looking up from liquid state enthalpy map as a function of pressure and temperature by using p_cond_actual and (T_cond_actual – subcool).

In order to calculate isentropic enthalpy at pump outlet (h2s), firstly, entropy at pump inlet (s1) is calculated by looking up from liquid state entropy map as a function of pressure and temperature by using p_cond_actual and (T_cond_actual – subcool). Isentropic enthalpy at pump outlet (h2s) is calculated by looking up from liquid state enthalpy map as a function of pressure and entropy by using p_evap_out and s1.

Enthalpy of working fluid at evaporator section where it begins to evaporate (h23a) is calculated from saturated liquid curve by using evaporation pressure (p_evap_out).

Working fluid enthalpy at expander inlet (h3) is calculated form vapor state enthalpy map as a function of pressure and temperature by using evaporation pressure (p_evap_out) and expander inlet temperature (T_evap+superheat).

In order to calculate isentropic enthalpy at expander outlet (h4s), firstly, entropy at expander inlet (s3) is calculated by looking up from vapor state entropy map as a function of pressure and temperature by using evaporation pressure (p_evap_out) and expander inlet temperature (T_evap+superheat). Isentropic enthalpy at expander outlet (h4s) is calculated by looking up from vapor state enthalpy map as a function of pressure and entropy by using condensation pressure (p_cond_actual) and entropy at expander inlet (s3).

Pump outlet temperature (T2) is calculated from liquid state enthalpy map as a function of pressure and enthalpy by using evaporation pressure (p_evap_out) and pump outlet enthalpy (h2).

Target condensation temperature (T_cond_target) is calculated from saturation vapor curve by using target condensation pressure (p_cond_target).

Enthalpy at condenser section where working fluid begins to condense (h41a) is calculated from saturation vapor curve by using actual condensation pressure (p_cond_actual).

2.1.1 COSMO fluid properties model

COSMO software predicts working fluid properties based on quantum chemistry and thermodynamics [16].

3D conformer files are downloaded from PubChem website for the working fluids. By using these 3D conformer files, maps for working fluid properties are created with COSMO software as a function of pressure and temperature. These maps are used to calculate working fluid properties by interpolation in Simulink (Figure 2.1).

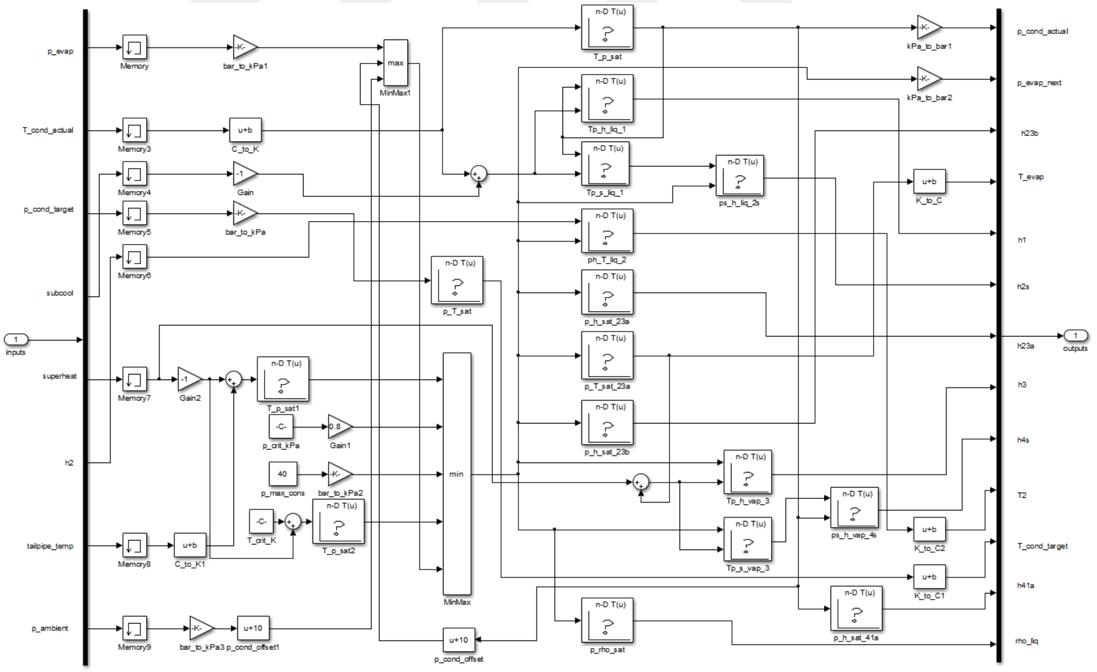

Figure 2.1 : COSMO fluid properties model in Simulink.

2.1.2 REFPROP fluid properties model

REFPROP program uses the most accurate equations available worldwide for the thermodynamic and transport properties to calculate the state points of the fluid or mixture [17]. REFPROP database is not directly used. It is used from GT-SUITE as

GT-SUITE also uses REFPROP database for fluid properties and GT-SUITE has a built-in template to lookup working fluid properties depending on pressure and temperature, which are calculated by the Rankine cycle model [18]. REFPROP fluid properties model is created in GT-SUITE (Figure 2.2) and the model is integrated with the Rankine cycle model in Simulink using GT-SUITE s-function.

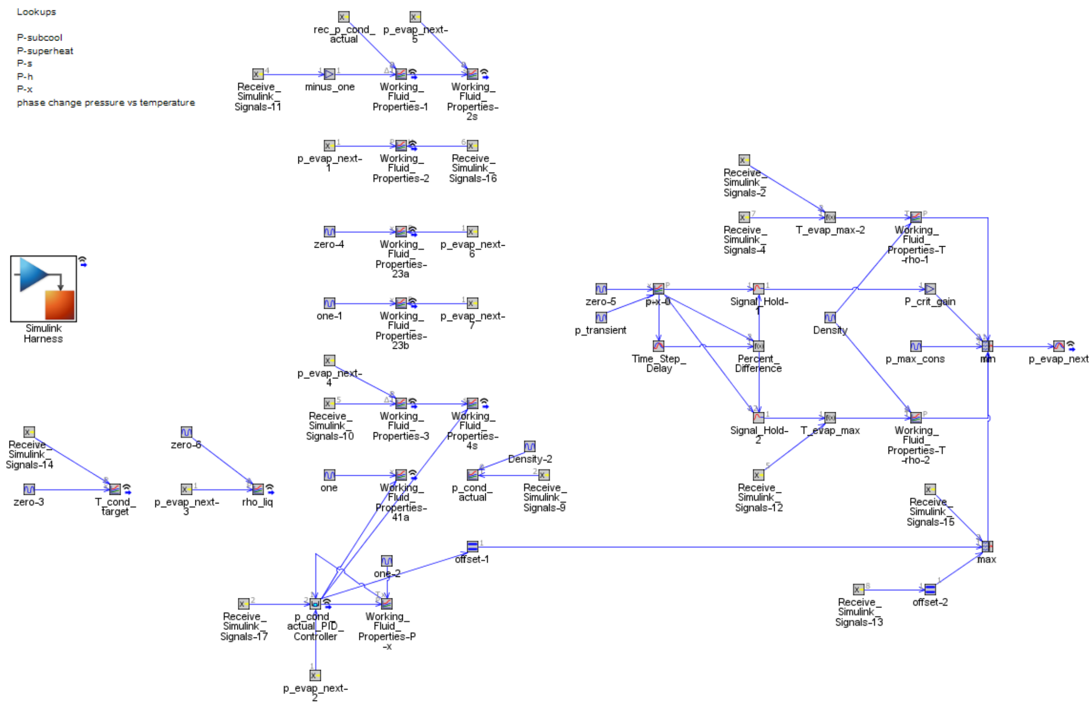

Figure 2.2 : REFPROP fluid properties model in GT-SUITE.

2.2 Rankine Cycle Model

Waste heat recovery system employs Rankine cycle to convert exhaust heat into useful work and hence improve fuel economy. Rankine cycle model calculates the heat transfer rates through evaporator and condenser, expander power, pump power, condensation and evaporation temperature, condensation and evaporation pressure, etc.

The inputs of the Rankine cycle model are pp_cond, cp_coolant, superheat, subcool, T_coolant_in_actual, T_cond_target, h41a, h1, wf_pump_eff, exp_eff, pp_evap, h_exh_in, h_exh_out, cp_exh, T_exh_out, T_exh_in, T_evap, h2s, h23a, h23b, h3, h4s, T2, air_flow, fuel_flow, p_evap_in. These inputs come from by fluid properties model, cooling model and test data.

The outputs of the Rankine cycle model are m_coolant_target, T_coolant_in_target, p_evap_out, P_exp, T_cond_actual, P_wf_pump, q_cond, h2, dT2, dT23a, dT23b, dT3, T_exh_out_next, m_wf. These outputs are used by fluid properties model and cooling model. Some of these outputs are also used to calculate fuel economy benefit.

Rankine cycle assumptions are given in Table 2.1.

Table 2.1 : Rankine cycle assumptions.

Parameter	Description	Unit	Assumption
pp_cond	Condenser pinch point	ºC	10
pp_evap	Evaporator pinch point	ºC	15
superheat	Evaporator outlet superheat	ºC	20
subcool	Condenser outlet subcool	ºC	10
exp_eff	Expander isentropic efficiency	%	60
wf_pump_eff	Pump isentropic efficiency	%	60

The numbering convention for the Rankine cycle calculations is given in Figure 2.3.

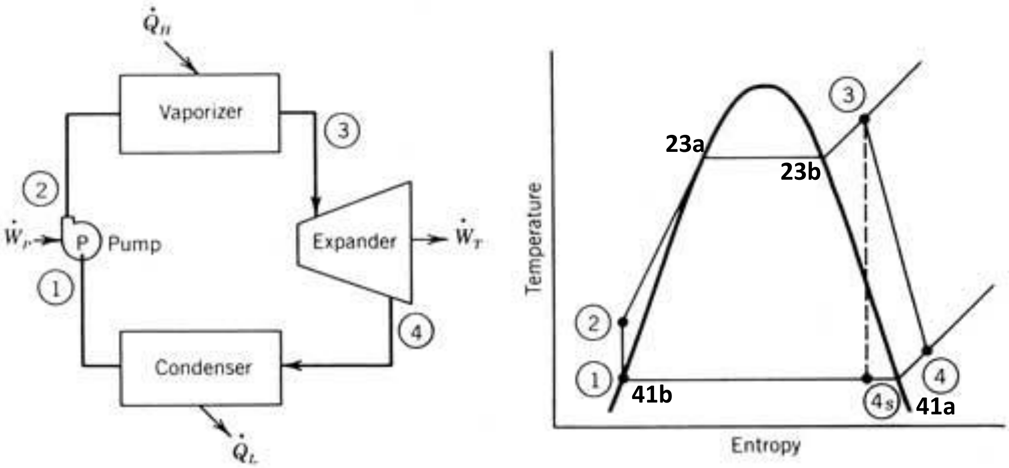

Figure 2.3 : The numbering convention for the Rankine cycle calculations.

The Rankine cycle model calculations are given in equations 1-21.

Heat transfer rate through evaporator:

$$q\_evap = m\_exh * (h\_exh\_in - h\_exh\_out) \tag{1}$$

Enthalpy at working fluid pump outlet:

$$h2 = \frac{(h2s - h1)}{wf\_pump\_eff} + h1 \tag{2}$$

Working fluid mass flow rate:

$$m\_wf = \frac{q\_evap}{h3 - h2} \tag{3}$$

Enthalpy at expander outlet:

$$h4 = h3 - \exp\_eff * (h3 - h4s) \tag{4}$$

Power generated by expander:

$$P\_exp = m\_wf * (h3 - h4) \tag{5}$$

Power consumed by working fluid pump:

$$P\_wf\_pump = m\_wf * (h2 - h1) \tag{6}$$

Heat transfer rate through condenser:

$$q\_cond = m\_wf * (h4 - h1) \tag{7}$$

Working fluid temperature at expander inlet:

$$T3 = T\_evap + superheat \tag{8}$$

Exhaust gas temperature in evaporator section where working fluid begins to evaporate:

$$T\_exh\_23a = T\_exh\_out + \frac{(m\_wf*(h23a - h2))}{m\_exh*cp\_exh} \tag{9}$$

Exhaust gas temperature in evaporator section where working fluid is fully evaporated:

$$T\_exh\_23b = T\_exh\_23a + \frac{(m\_wf*(h23b - h23a))}{m\_exh*cp\_exh} \tag{10}$$

Pinch point temperature difference at evaporator inlet:

$$dT2 = T\_exh\_out - T2 \tag{11}$$

Pinch point temperature difference in evaporator section where working fluid begins to evaporate:

$$dT23a = T\_exh\_23a - T\_evap \tag{12}$$

Pinch point temperature difference in evaporator section where working fluid is fully evaporated:

$$dT23b = T\_exh\_23b - T\_evap \tag{13}$$

Pinch point temperature difference at evaporator outlet:

$$dT3 = T\_exh\_in - T3 \tag{14}$$

Minimum of pinch point differences:

$$dTmin = \min(dT23a, dT23b, dT3) \tag{15}$$

Evaporation pressure at next time step to maintain target *pp_evap*:

$$p\_evap\_out = p\_evap\_in + 0.1 * (dTmin - pp\_evap) \tag{16}$$

Exhaust gas temperature at evaporator outlet at next time step to maintain target 4* *pp_evap*:

$$T\_exh\_out\_next = T\_exh\_out - 0.1 * (dT2 - 4 * pp\_evap) \tag{17}$$

Actual condensation temperature at next time step:

$$T\_cond\_actual = T\_coolant\_in\_actual + pp\_cond + subcool \tag{18}$$

Target coolant temperature at condenser section where working fluid begins to condense:

$$T\_41a\_coolant\_target = T\_cond\_target - pp\_cond \tag{19}$$

Target coolant temperature at condenser inlet:

$$T\_coolant\_in\_target = T\_cond\_target - subcool - pp\_cond \tag{20}$$

Target coolant flow rate:

$$m\_coolant\_target = \frac{m\_wf * (h41a - h1)}{cp\_coolant * (T\_41a\_coolant\_target - T\_coolant\_in\_target)} \tag{21}$$

2.3 Cooling System Model

Cooling system model is created in GT-SUITE (Figure 2.4). The model consists of coolant pump, condenser, radiator and fan.

The pump object imposes specified flow rate ($m\_coolant\_target$) that is calculated by the Rankine cycle model. The efficiency of the coolant pump is assumed as 60%.

The condenser is modeled with pressure drop and heat rejection data. Pressure drop across the condenser is assumed as 0.2 bar at 140 L/min coolant flow rate. Condenser heat rejection (q_cond) is calculated by the Rankine cycle model and it is imposed on the coolant.

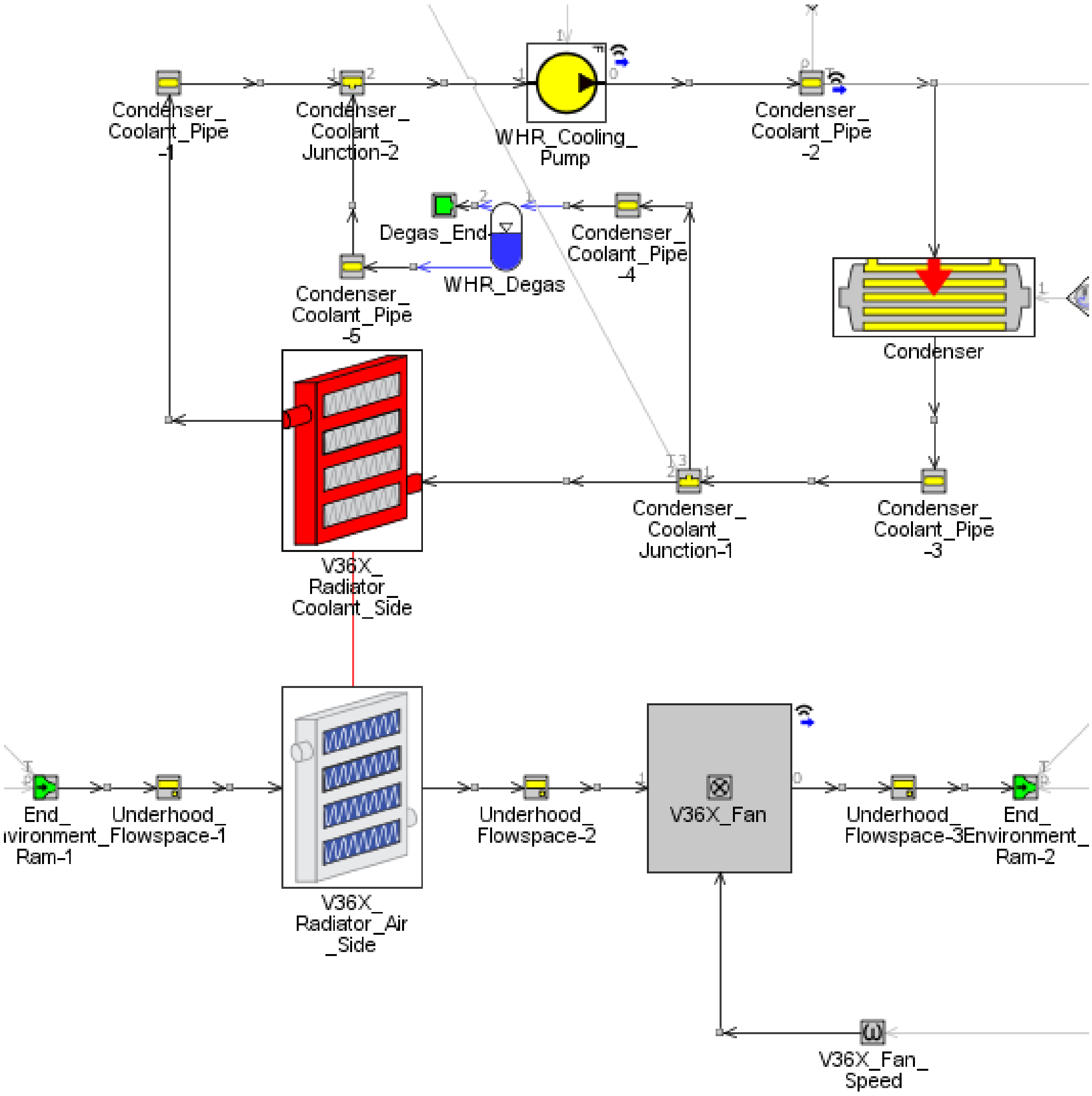

Figure 2.4 : Cooling system model in GT-SUITE.

The radiator is modeled with heat transfer data and pressure drop data of coolant side and airside. Heat transfer data is entered depending on coolant flow rate, coolant inlet temperature, airflow rate, air inlet temperature.

The fan is modeled with performance data that includes pressure rise and efficiency depending on flow rate at different speeds. Fan speed is controlled to maintain target coolant temperature at condenser inlet($T\_coolant\_in\_target$).

End environment objects are used to impose ambient pressure and ambient temperature. Generic piping is used to connect the parts in the cooling system.

2.4 Transient Cycle Data

A transient vehicle test data is used to carry out simulations. The following data is taken from test: engine speed, brake torque, air mass flow rate, fuel mass flow rate, tailpipe temperature, ambient pressure and ambient temperature.

Engine speed and brake torque is used to calculate engine brake power. Engine brake power is used to calculate fuel economy benefit.

The sum of air mass flow rate and fuel mass flow rate is used as exhaust mass flow rate flowing through evaporator.

Tailpipe temperature is used as gas temperature at evaporator inlet.

Ambient pressure and ambient temperature are used as boundary condition in the cooling system model. Ambient pressure is also used as target condensation pressure to prevent air leakage into the Rankine cycle.

2.5 Integrated Model

All the models (fluid properties model (COSMO or REFPROP), Rankine cycle model (Matlab function), and GT-SUITE cooling model) are integrated in a Simulink model and connections between models are created. GT-SUITE s-function in Simulink library is used to enable combined GT-SUITE – Simulink simulation. Fuel economy benefit is calculated in the integrated Simulink model by dividing cumulative net power by cumulative engine brake power.

COSMO integrated model is depicted in Figure 2.5 and REFPROP integrated model is depicted in Figure 2.6. The major difference between two integrated models is the calculation way of fluid properties.

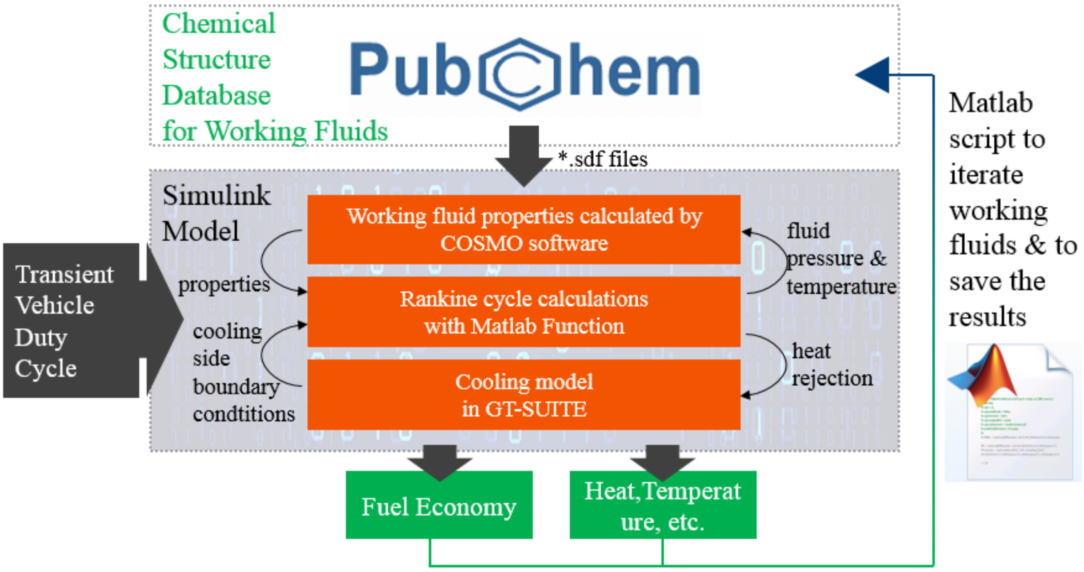

Figure 2.5 : Integrated model for COSMO simulations.

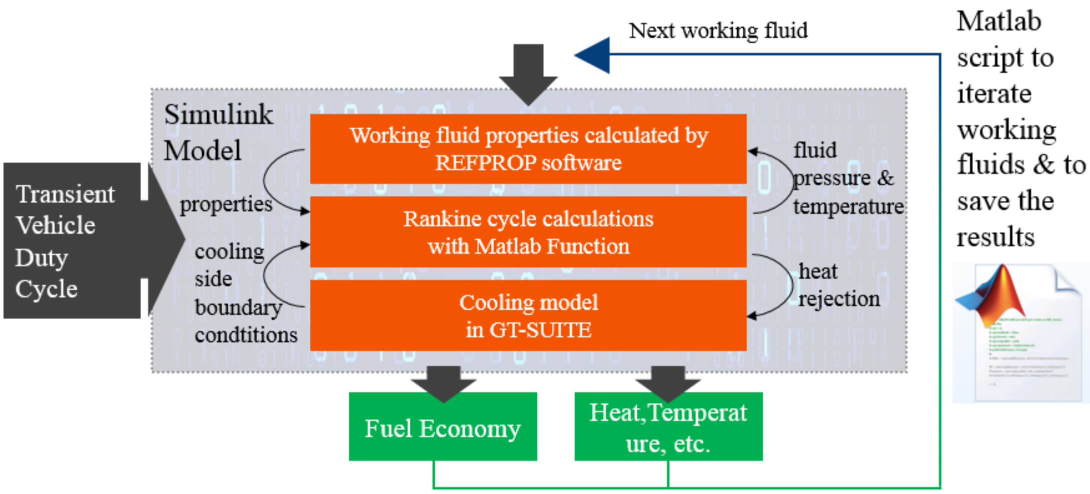

Figure 2.6 : Integrated model for REFPROP simulations.

2.6 Script to Run Working Fluid Iterations and to Save the Results

Two Matlab scripts (*.m files) are written to run the integrated model and to print the results to an Excel file for each working fluid iteratively. Matlab scripts are different for COSMO and REFPROP fluid properties models. The Matlab script for the REPFROP model runs the integrated model and prints the results. The Matlab script for the COSMO model additionally generates tables of output values by using maps generated by the COSMO software for each working fluid. The COSMO properties model uses these tables to calculate fluid properties by interpolation.

2.7 Simulated Working Fluids

Simulations are carried out for 146 working fluids. 31 working fluids are assessed by using both COSMO and REFPROP softwares. 98 working fluids are assessed by using only COSMO since they are not available in REFPROP database. 17 working fluids are assessed by using only REFPROP since COSMO failed to calculate the properties for these working fluids ().

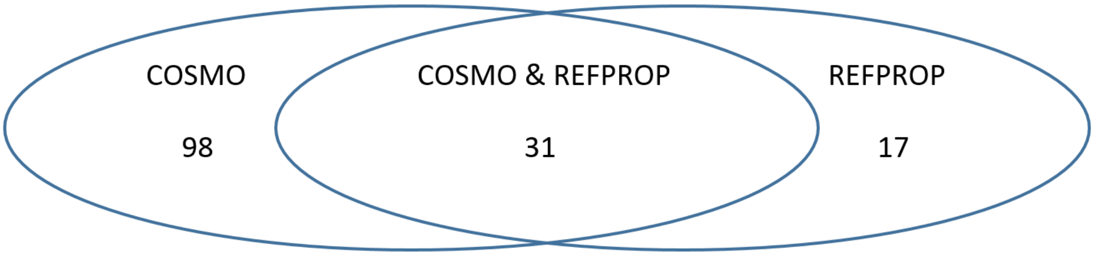

Figure 2.7 : The number of simulated working fluids.

3. SIMULATION RESULTS

Simulation results are reported for transient cycle and for steady state cruise condition. Firstly, the results and the working fluid ranking with REFPROP software are reported for transient cycle and for steady state condition. The results are reported for cyclopentane, ethanol, R245fa, and water are reported in more detail as they are the most studied working fluids in the literature. Secondly, the resultsand the working fluid ranking with COSMO software are reported. At the end, working fluid ranking results with REFPROP and COSMO softwares are compared.

3.1 Simulation Inputs

The following inputs are used in the transient cycle simulations and they are taken from test data: airflow rate, brake torque, engine speed, fuel flow rate, tailpipe temperature.

Airflow rate is used to calculate exhaust mass flow rate (Figure 3.1).

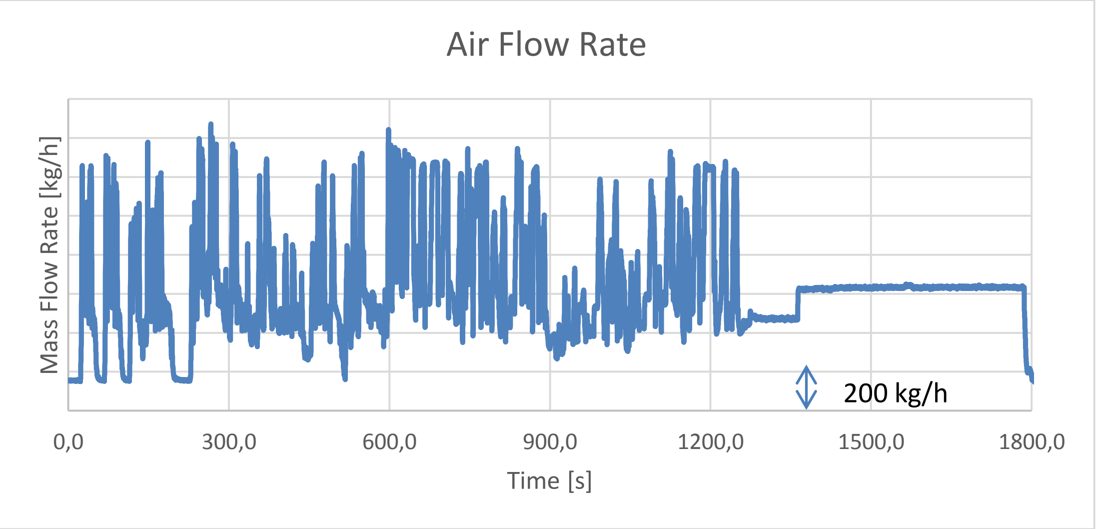

Figure 3.1 : Air flow rate.

Fuel flow rate is also used to calculate exhaust mass flow rate (Figure 3.2).

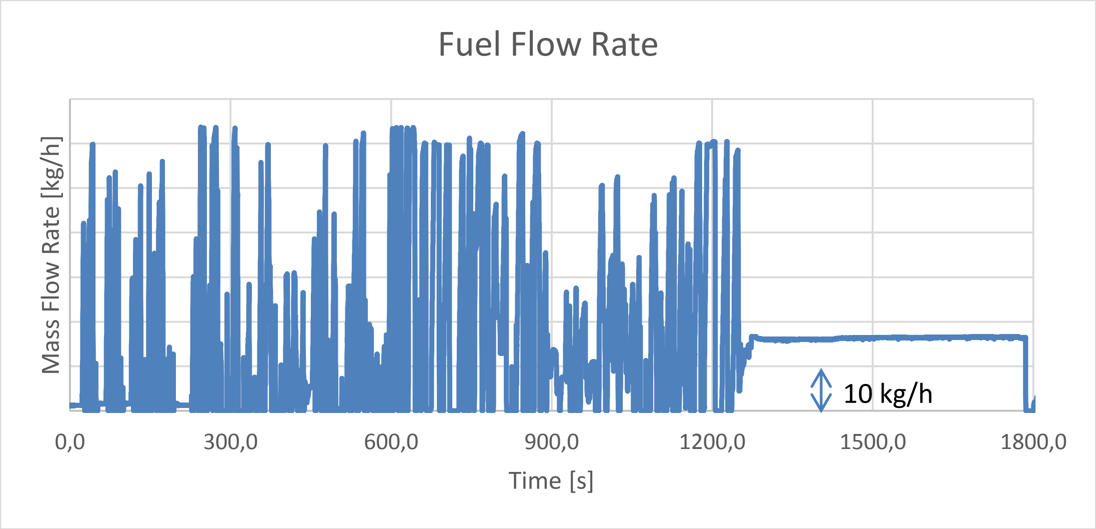

Figure 3.2 : Fuel flow rate.

Brake torque is used to calculate engine brake power (Figure 3.3). Cumulative brake power is used to calculate cumulative fuel economy benefit.

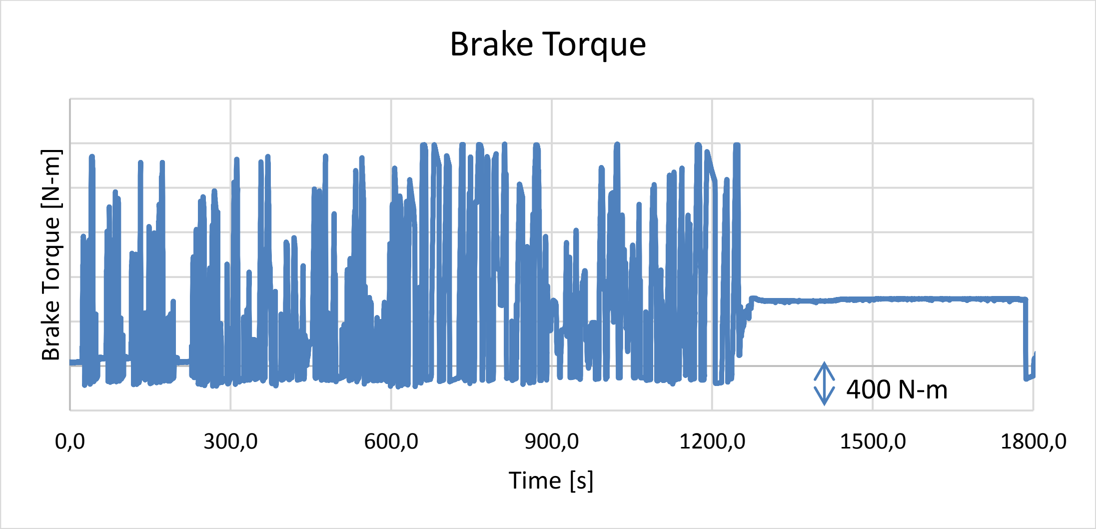

Figure 3.3 : Brake torque.

Engine speed is also used to calculate engine brake power (Figure 3.4). Cumulative brake power is used to calculate cumulative fuel economy benefit.

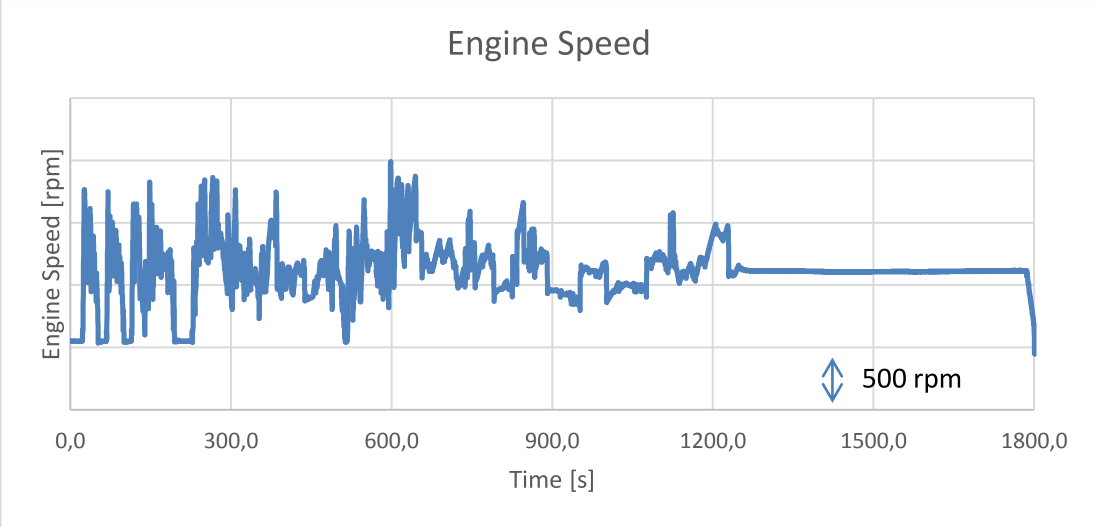

Figure 3.4 : Engine speed.

Tailpipe temperature is used to calculate evapor ation pressure (Figure 3.5).

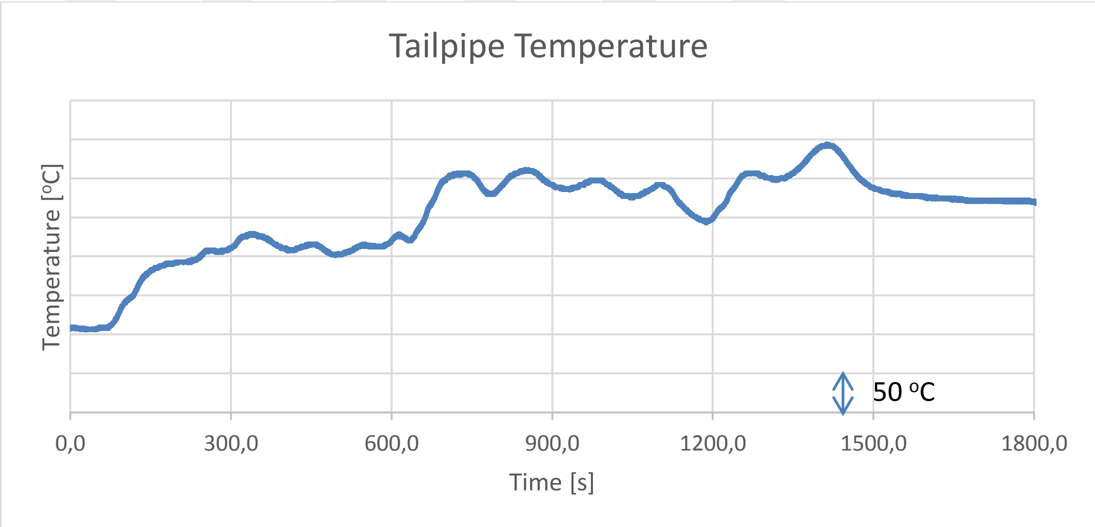

Figure 3.5 : Tailpipe temperature.

3.2 Simulation Results with REFPROP

Simulations are carried out with working fluid properties calculated by REFPROP software. Simulations are carried out for 48 working fluids.

3.2.1 Working fluid ranking with REFPROP

Simulation results show that cyclopentane has the highest fuel economy benefit. Ethanol is the 8th in the ranking. Some of the working fluids have negative fuel economy benefit because it is not possible to condense these working fluids at the specified ambient temperature (Figure 3.6).

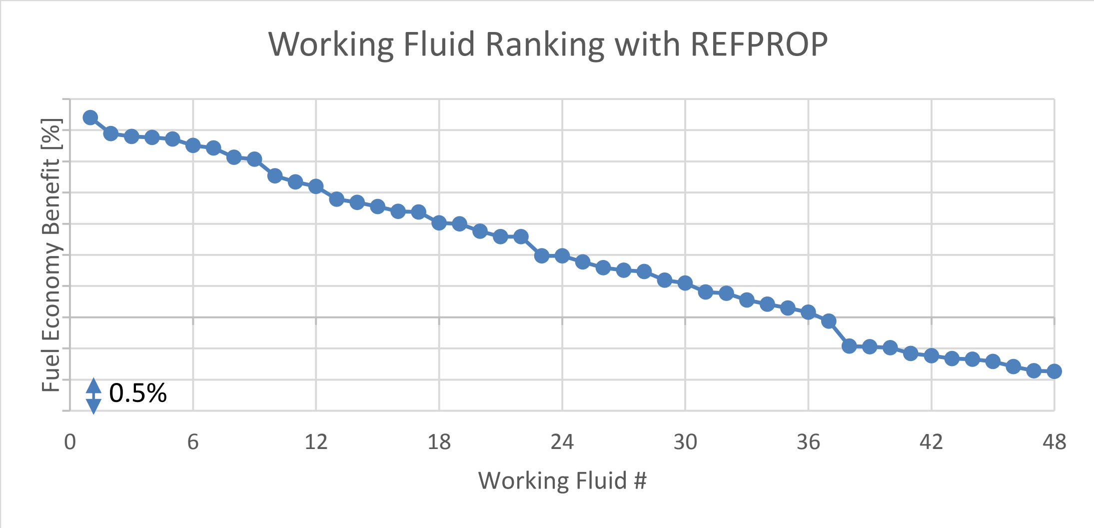

Figure 3.6 : Working fluid ranking with REFPROP.

3.2.2 Other results for 48 working fluids

Simulation results show that there is not a correlation between fuel economy benefit and evaporation pressure. Evaporation pressure is limited by 40 bar due to structural reasons (Figure 3.7).

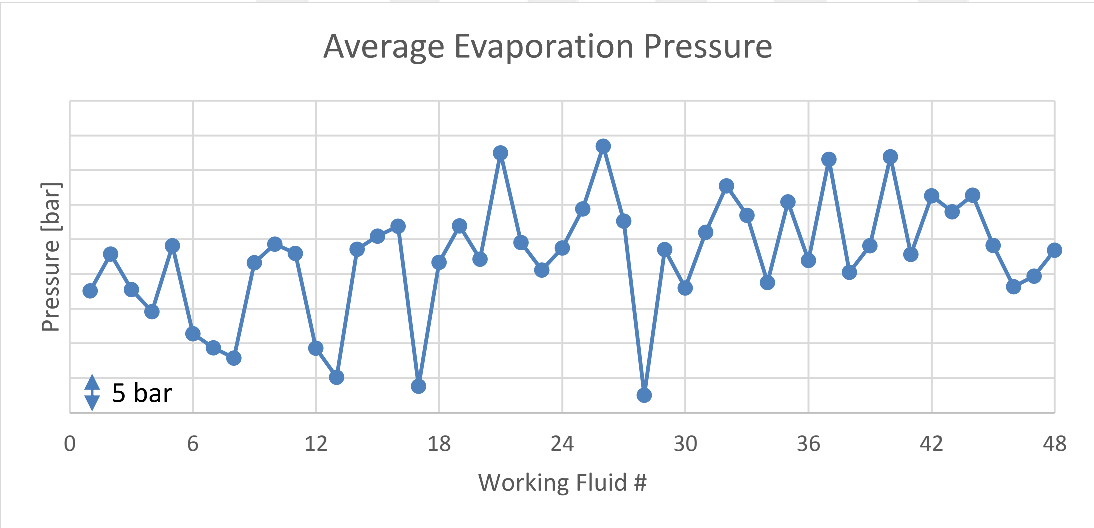

Figure 3.7 : Average evaporation pressure.

Simulation results show that working fluids with higher fuel economy ranking have also high evaporation temperature (Figure 3.8).

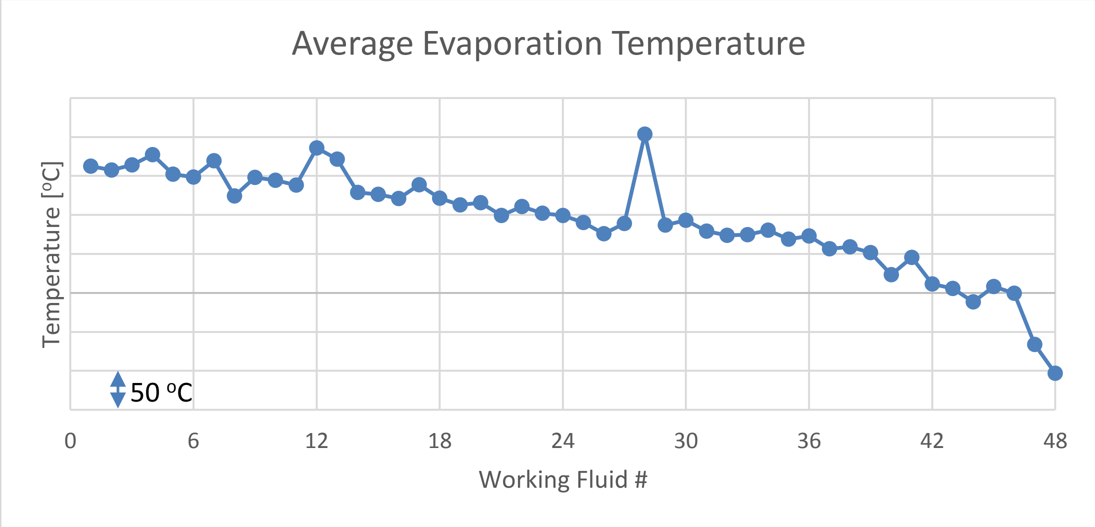

Figure 3.8 : Average evaporation temperature.

Simulation results show that fan operates at maximum speed for most of the working fluids in order to maintain 1.0 bar target condensation pressure. This means that condensation temperature at 1.0 bar is very low for these working fluids (Figure 3.9).

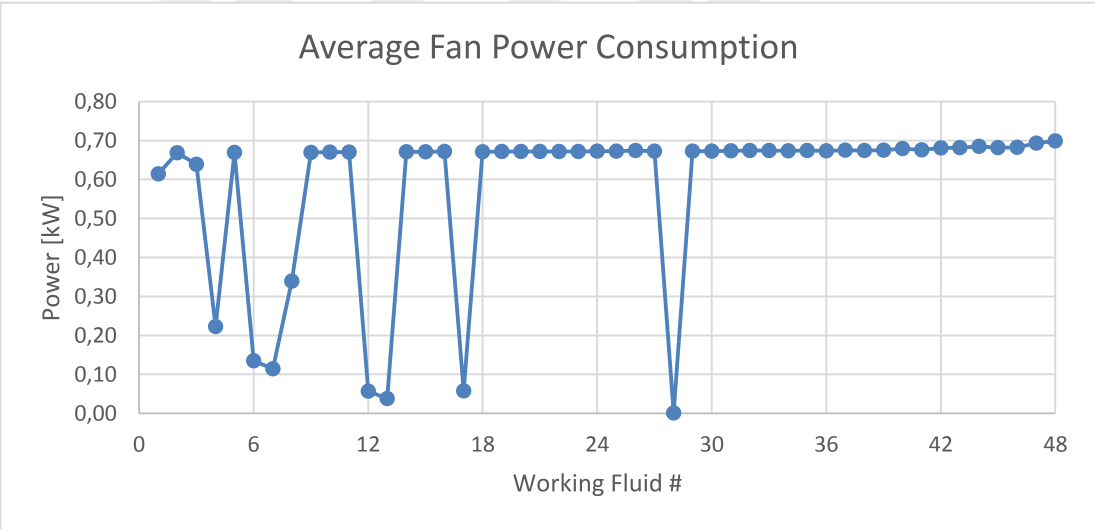

Figure 3.9 : Average fan power consumption.

Simulation results show that condensation temperature is around 60 ºC when fan operates at maximum speed for most of the working fluids. Condensation temperature is higher than 60 ºC when fan does not need to operate at maximum speed to maintain 1.0 bar target condensation pressure.

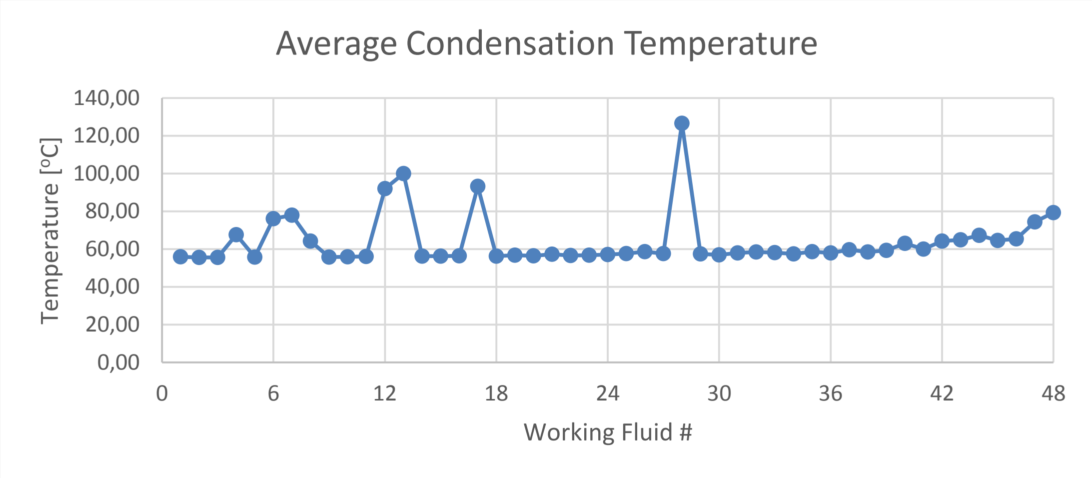

Figure 3.10 : Average condensation temperature.

Simulation results show that for most of the working fluids it is not possible to maintain 1.0 bar target condensation pressure although fan operates at maximum speed. It is also shown that working fluids, which have low FE benefit ranking, have high condensation pressure (Figure 3.11).

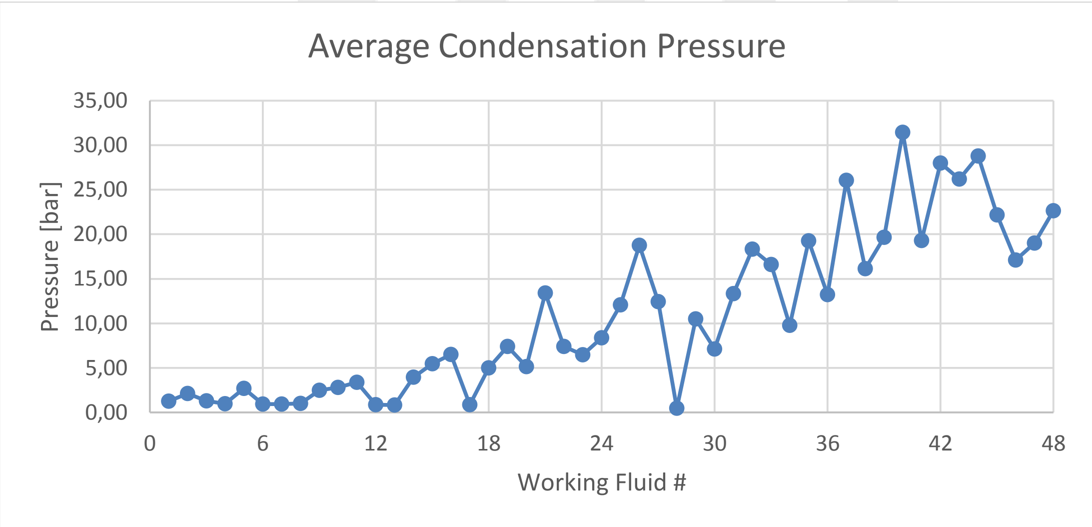

Figure 3.11 : Average condensation pressure.

3.2.3 Steady state results at cruise operation point for cyclopentane, ethanol, R245fa, and water

Steady state simulation results are reported for some of the working fluids. These working fluids are cyclopentane, ethanol, R245fa, and water. These working fluids are selected because they are the most studied fluids in literature.

Steady state simulation results show that cyclopentane has the highest net power output due to the highest evaporation temperature. Cyclopentane has the highest evaporator heat rate due to the lowest condensation temperature (low evaporator inlet temperature). R245fa has the highest pump power input due to the highest mass flow rate. R245fa has the highest mass flow rate due to the lowest entropy difference during phase change (the lowest T-s diagram area). Cyclopentane has the highest evaporation temperature due to the high heat capacity rate and high critical point. Cyclopentane has the highest evaporation pressure due to the highest evaporation temperature (Table 2.2).

Table 2.2 : Steady state simulation results.

Parameter	Unit	Cyclop entane	Ethanol	R245fa	Water
Evaporator Heat Rate	kW	32.40	28.31	31.96	24.09
Condenser Heat Rate	kW	28.83	25.82	29.63	22.56
Pump Power Input	kW	0.19	0.06	0.34	0.01
Expander Power Output	kW	3.76	2.55	2.66	1.53
Net Power Output	kW	3.57	2.50	2.33	1.53
Working Fluid Mass Flow Rate	kg/s	0.0553	0.0281	0.1255	0.0100
Evaporation Pressure	bar	16.0	10.0	25.0	4.3
Condensation Pressure	bar	1.3	1.0	4.5	1.0
Evaporation Temperature	ºC	168.0	150.7	133.4	146.6
Condensation Temperature	ºC	57.0	78.1	58.7	99.6
Thermal Efficiency	%	11.0	8.8	7.3	6.3
Specific Heat	kJ/kg-K	2.29	3.30	1.56	4.24
Heat Capacity Rate	kW/K	0.1268	0.0929	0.1958	0.0424

3.2.3.1 Steady state results at cruise operation point for cyclopentane

In T-q diagram of cyclopentane, it can be clearly seen that pre-heating grade is very low due to high heat capacity rate. As a result, evaporation temperature becomes very high when compared to other working fluids (Figure 3.12).

In T-s diagram of cyclopentane, it can be clearly seen that a recuperator can be used to further increase fuel economy benefit because superheat at expander outlet is very high since it is a dry fluid (Figure 3.13).

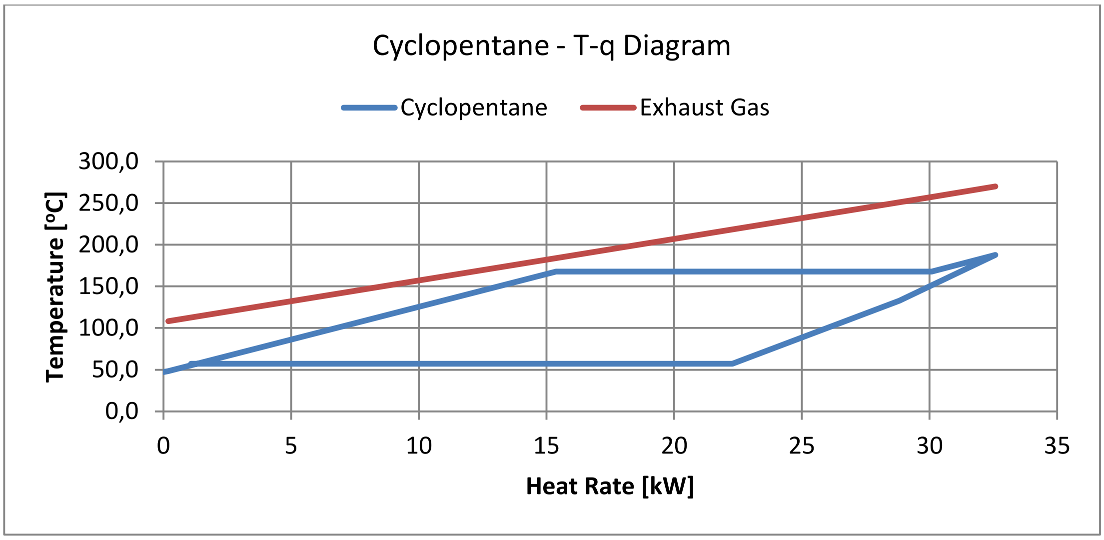

Figure 3.12 : T-q diagram for cyclopentane.

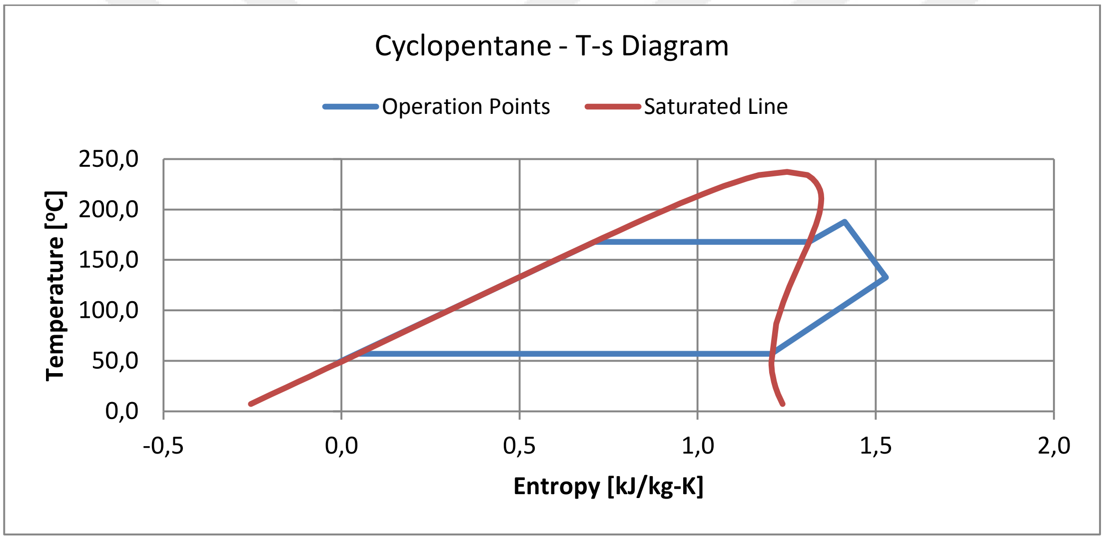

Figure 3.13 : T-s diagram for cyclopentane.

3.2.3.2 Steady state results at cruise operation point for ethanol

In T-q diagram of ethanol, it can be seen that its pre-heating grade is higher than that of cyclopentane due to lower heat capacity rate. As a result, it has lower evaporation temperature due to pinch point temperature difference limitation, lower thermal efficiency, and lower net power output (Figure 3.14).

In T-s diagram of ethanol, it can be seen that it has higher operation point area due to higher entropy difference during phase change when compared to cyclopentane. As a result, it has lower working fluid mass flow rate than cyclopentane (0.0553 kg/s with cyclopentane vs. 0.0281 kg/s with ethanol). It can also be seen that superheat at expander outlet is very low since ethanol is a wet fluid. As a result, using a recuperator is not going to increase fuel economy benefit (Figure 3.15).

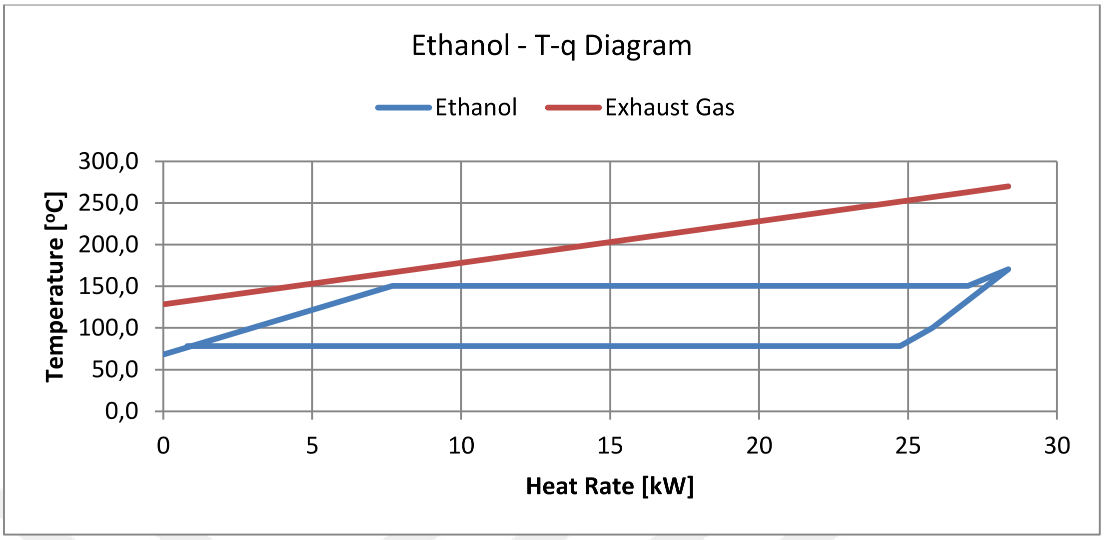

Figure 3.14 : T-q diagram for ethanol.

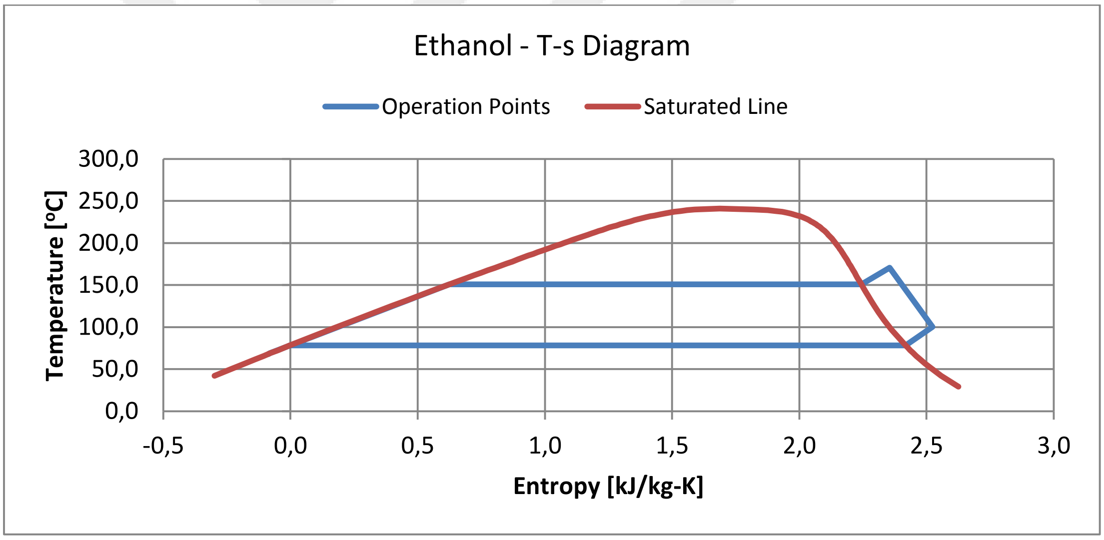

Figure 3.15 : T-s diagram for ethanol.

3.2.3.3 Steady state results at cruise operation point for R245fa

In T-q diagram of R245fa, it can be seen that evaporation temperature is not limited by pinch point difference limitation since it has the highest heat capacity rate (0.1958 kW/K with R245fa vs. 0.1268 kW/K with cyclopentane). Evaporation temperature is limited because evaporator outlet temperature is limited by the critical temperature (153 ^{o}C) (Figure 3.16).

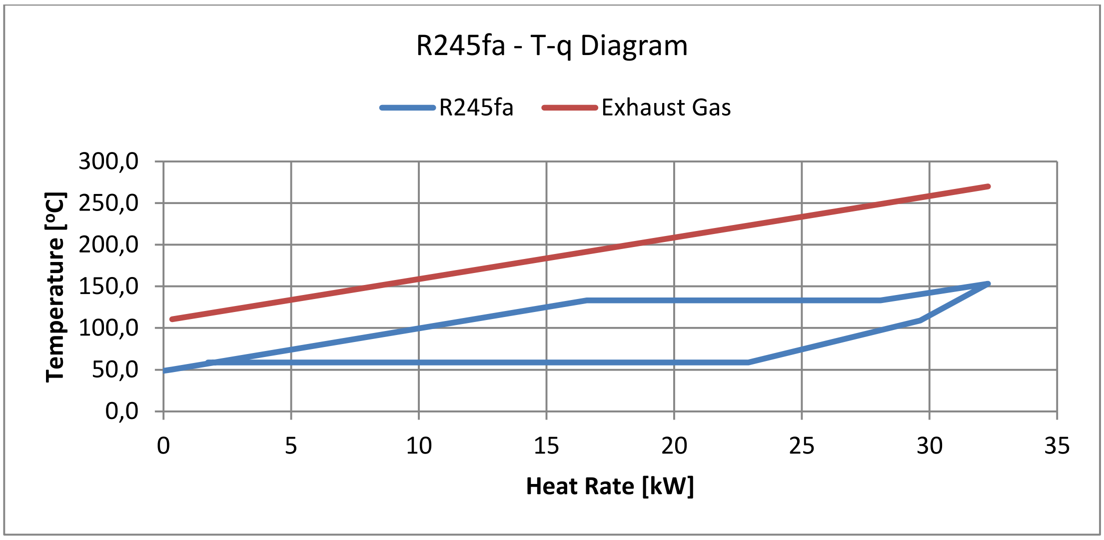

Figure 3.16 : T-q diagram for R245fa.

In T-s diagram of R245fa, it can be seen that it has lower operation point area due to lower entropy difference during phase change when compared to cyclopentane. As a result, it has higher working fluid mass flow rate than cyclopentane (0.0553 kg/s with cyclopentane vs. 0.1255 kg/s with R245fa). It can also be seen that a recuperator can be used to further increase fuel economy benefit because superheat at expander outlet is very high since it is also a dry fluid like cyclopentane (Figure 3.17).

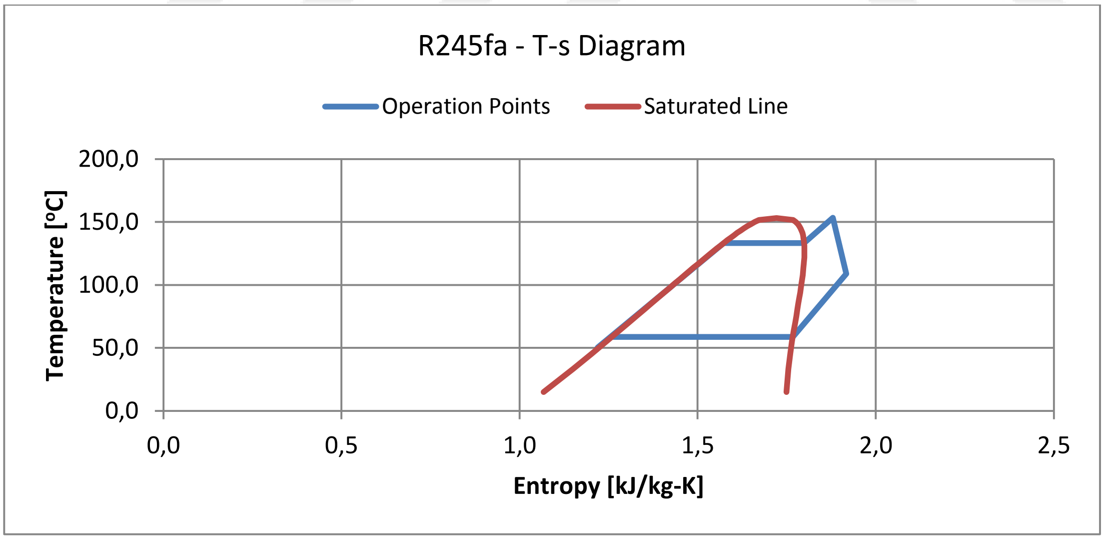

Figure 3.17 : T-s diagram for R245fa.

3.2.3.4 Steady state results at cruise operation point for water

In T-q diagram of water, it can be seen that its pre-heating grade is higher than that of cyclopentane due to lower heat capacity rate. As a result, it has lower evaporation temperature due to pinch point temperature difference limitation, lower thermal efficiency, and lower net power output (Figure 3.18).

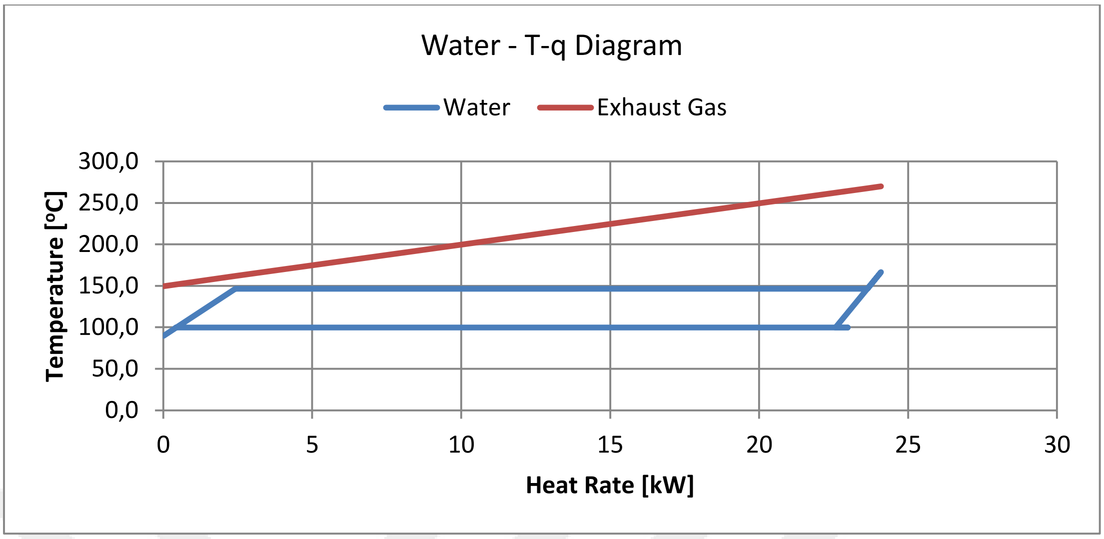

Figure 3.18 : T-q diagram for water.

In T-s diagram of water, it can be seen that it has higher operation point area due to higher entropy difference during phase change when compared to cyclopentane. As a result, it has lower working fluid mass flow rate than cyclopentane (0.0553 kg/s with cyclopentane vs. 0.0100 kg/s with water). It can also be seen that water at expander outlet is saturated since it is a wet fluid. As a result, using a recuperator is not going to increase fuel economy benefit for water (Figure 3.19).

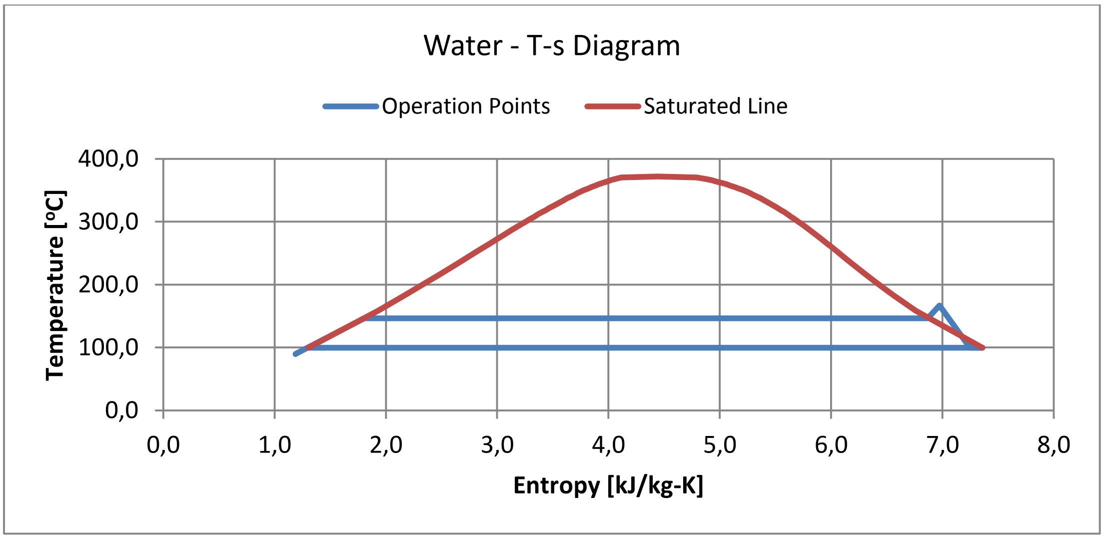

Figure 3.19 : T-s diagram for water.

3.2.4 Transient simulation results with REFPROP

Transient simulation results are also reported for cyclopentane, ethanol, R245fa, and water.

Cycle average results are reported in the following table (Table 2.3).

Table 2.3 : Transient cycle average simulation results.

Parameter	Unit	Cyclop entane	Ethanol	R245fa	Water
Evaporator Heat Rate	kW	28.52	24.95	28.70	21.64
Condenser Heat Rate	kW	25.37	22.61	26.58	20.24
Pump Power Input	kW	0.21	0.07	0.30	0.01
Expander Power Output	kW	3.36	2.40	2.42	1.41
Net Power Output	kW	2.57	2.19	1.48	1.34
Working Fluid Mass Flow Rate	kg/s	0.0483	0.0246	0.1120	0.0089
Evaporation Pressure	bar	17.7	11.4	23.6	3.8
Condensation Pressure	bar	1.27	0.94	4.01	0.87
Evaporation Temperature	ºC	162.8	148.6	128.9	139.3
Condensation Temperature	ºC	56.4	76.2	56.7	93.7
Thermal Efficiency	%	9.0	8.8	5.2	6.2
Fan Speed	rpm	2847	1385	2994	951
FE Benefit	%	3.23	2.75	1.87	1.68
Coolant Pump Power Input	kW	0.007	0.010	0.008	0.008
Fan Power Input	kW	0.575	0.138	0.631	0.059

Results of fuel economy benefit show that cyclopentane has the highest fuel economy benefit in transient cycle also because it has the highest cycle average evaporation temperature (Figure 3.20).

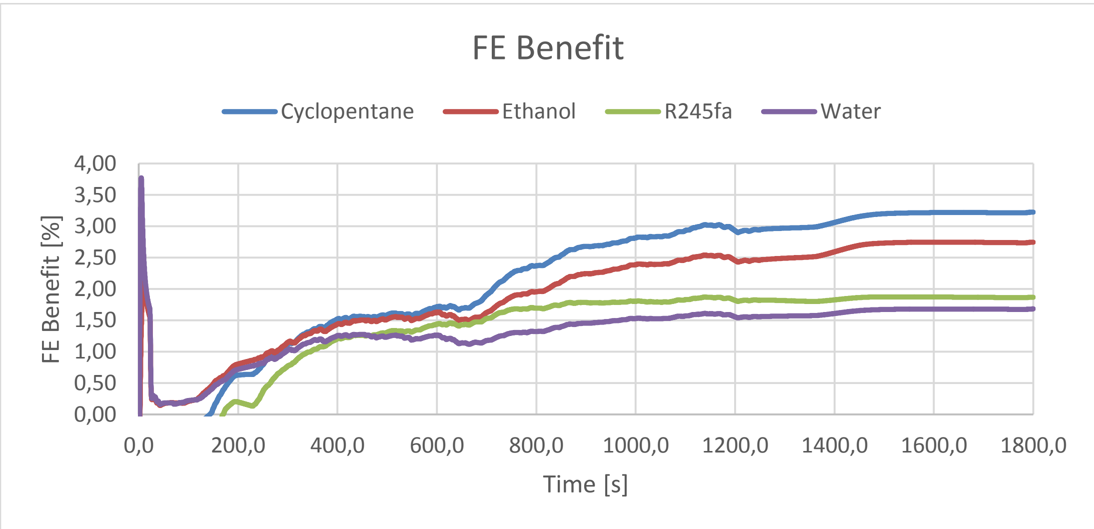

Figure 3.20 : Cumulative FE benefit results in transient cycle.

Net power generation results show that cyclopentane has the highest net power generation also again due to the highest cycle average evaporation temperature (Figure 3.21).

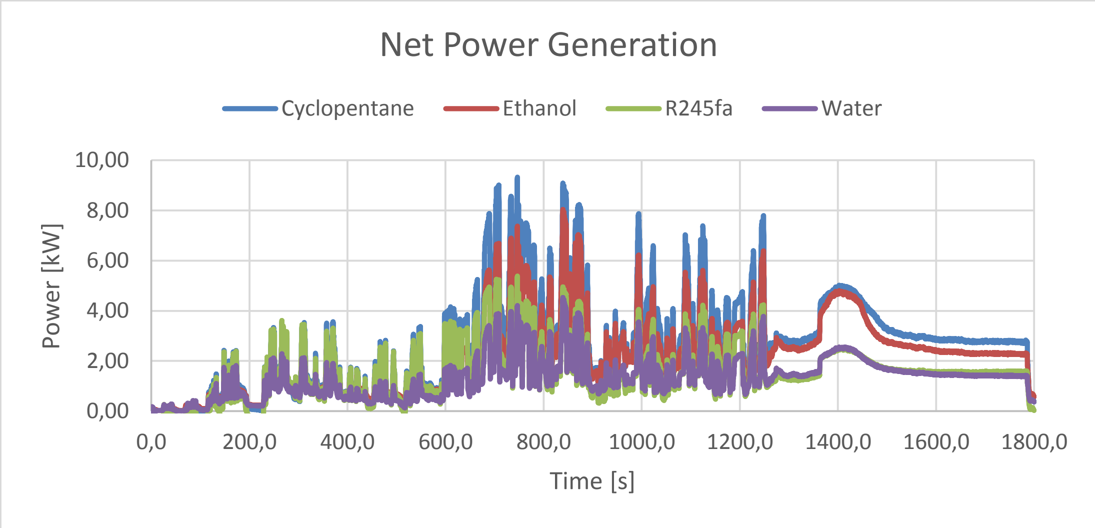

Figure 3.21 : Net power generation in transient cycle.

Cyclopentane has the highest expander power again due to the highest evaporation temperature (Figure 3.22).

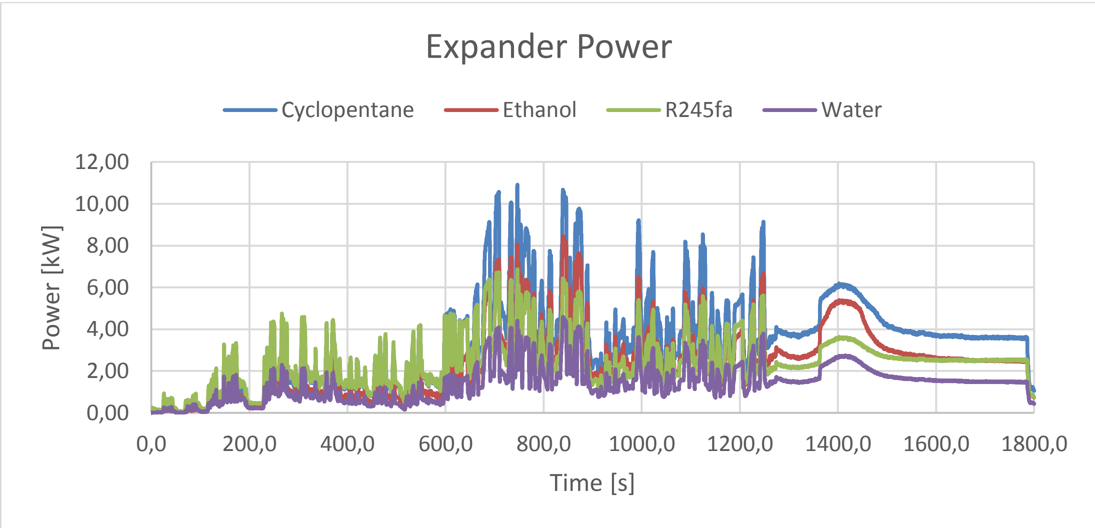

Figure 3.22 : Expander power output in transient cycle.

Evaporation temperature results show that cyclopentane has the highest cycle average evaporation temperature because it has the highest heat capacity rate except for R245fa. R245fa evaporation temperatur is lower than cyclopentane although it has higher heat capacity rate due to low critical temperature (Figure 3.23).

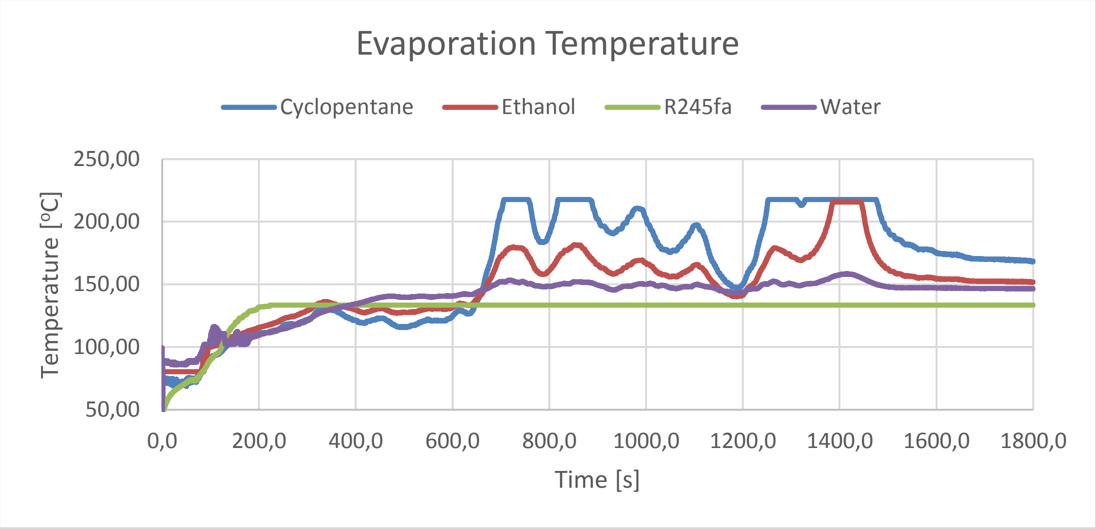

Figure 3.23 : Evaporation temperature in transient cycle.

Evaporation pressure results show that R245fa has the highest cycle average evaporation pressure because it has the highest heat capacity rate (Figure 3.24).

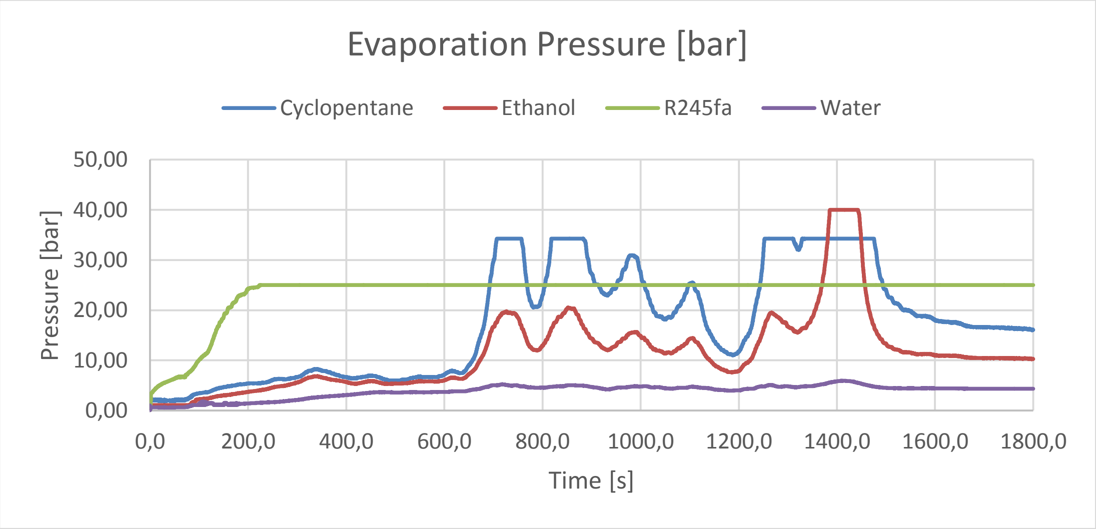

Figure 3.24 : Evaporation pressure in transient cycle.

Fan speed results show that R245fa has the highest cycle average fan speed because it has the lowest condensation temperature at 1.0 bar target condensation pressure. Fan operates at 3000 rpm limit for cyclopentane and R245fa because it is not possible to maintain target condensation temperature at 1.0 bar pressure with 20 ^{o}C ambient temperature (Figure 3.25). As a result, it is not possible to maintain 1.0 bar target condensation pressure for R245fa and cyclopentane (Figure 3.26).

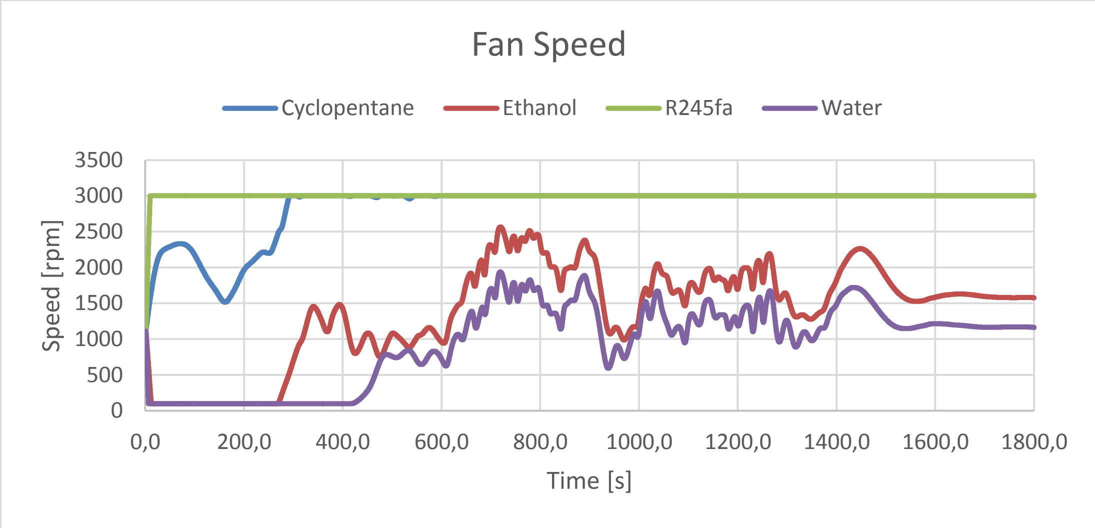

Figure 3.25 : Fan speed in transient cycle.

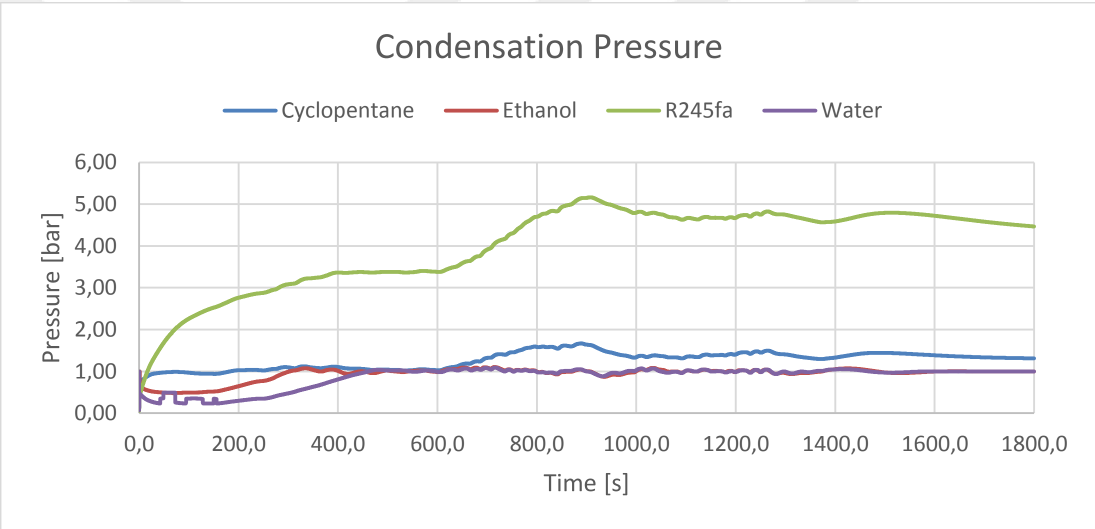

Figure 3.26 : Condensation pressure in transient cycle.

Target condensation temperature for water and ethanol is achieved due to higher condensation temperature. Target condensation temperature cannot be achieved for cyclopentane and R245fa due to very low target condensation temperature at 1.0 bar. Since fan is operating at 3000-rpm limit for cyclopentane and R245fa, their actual condensation temperatures are very close to each other (Figure 3.27).

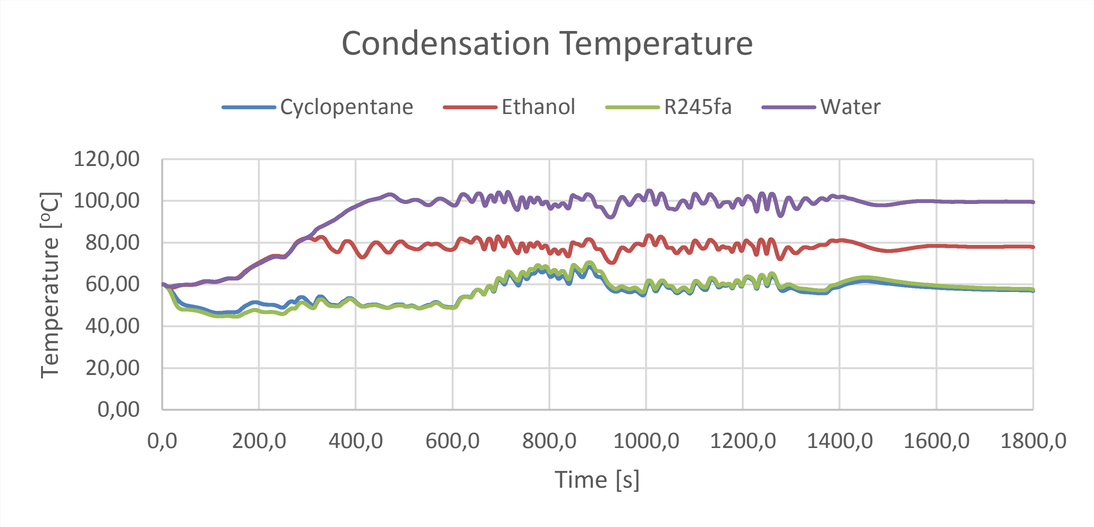

Figure 3.27 : Condensation temperature in transient cycle.

Fan power is proportional to fan speed and it is the highest for R245fa due to very low target condensation temperature at 1.0 bar target condensation pressure (Figure 3.28).

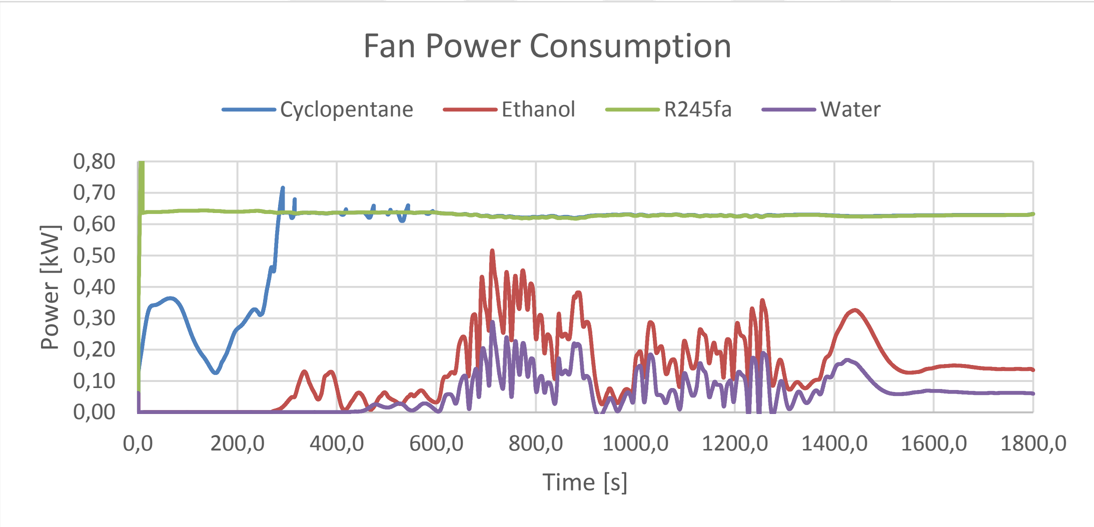

Figure 3.28 : Fan power consumption in transient cycle.

Working fluid mass flow rate results show that R245fa has the highest cycle average mass flow rate because it has the lowest entropy difference during phase change (the lowest T-s operation area) (Figure 3.29).

Results for working fluid volume flow rate show that R245fa has the highest cycle average volume flow rate because it has the highest cycle average mass flow rate (Figure 3.30).

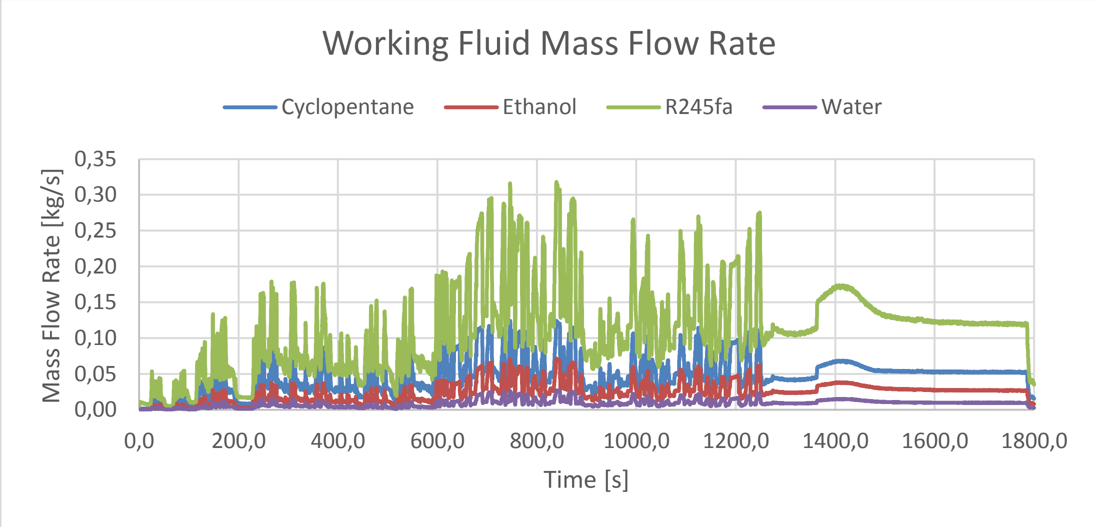

Figure 3.29 : Working fluid mass flow rate in transient cycle.

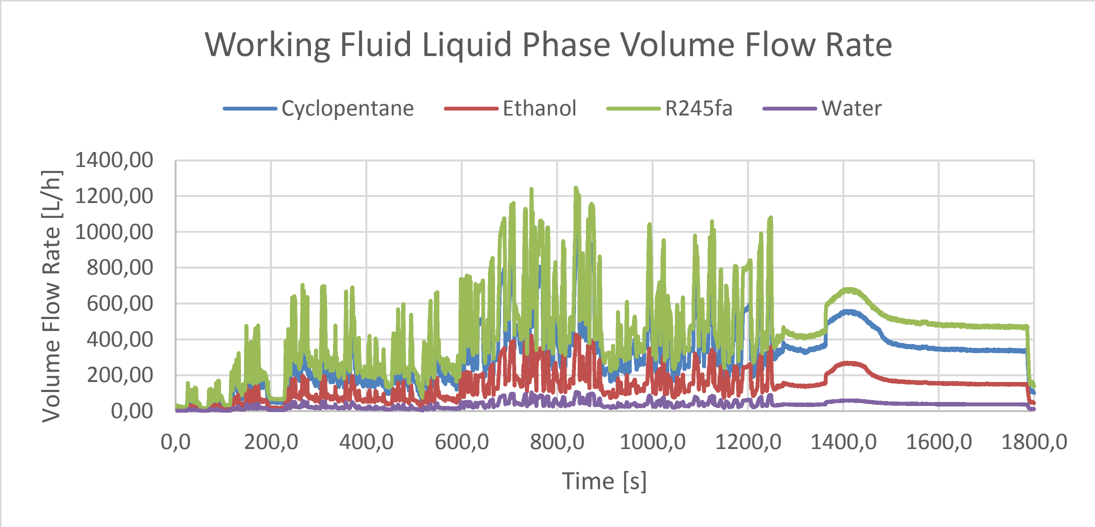

Figure 3.30 : Working fluid volume flow rate in transient cycle.

Working fluid pump power consumption is the highest with R245fa due to very high mass flow rate and pressure rise (Figure 3.31).

Power consumption of coolant pump results are very close to each other for all of the working fluids (Figure 3.32).

Water has the lowest cycle average evaporator heat transfer rate due to the highest condensation temperature (the highest evaporator inlet temperature) (Figure 3.33).

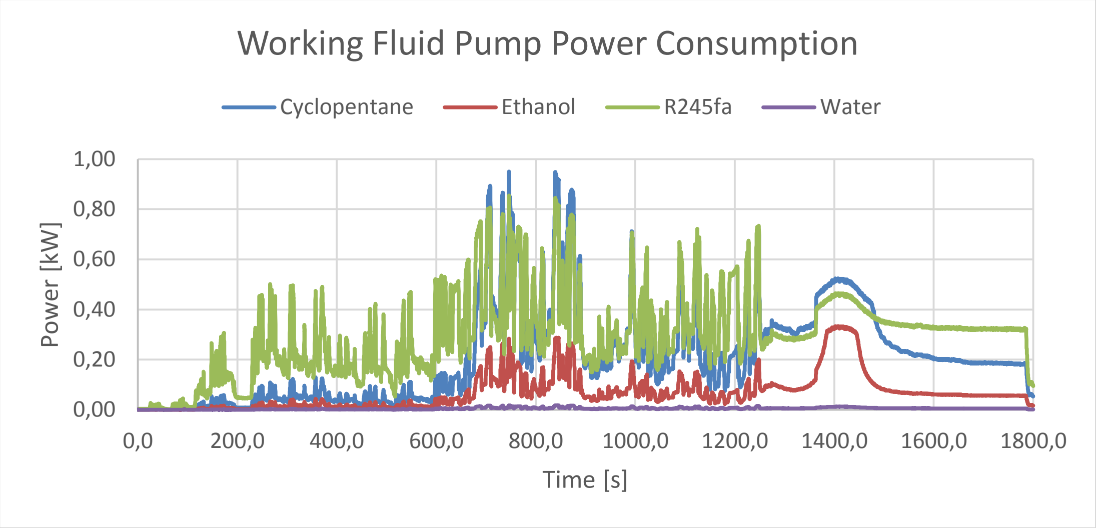

Figure 3.31 : Working fluid pump power consumption in transient cycle.

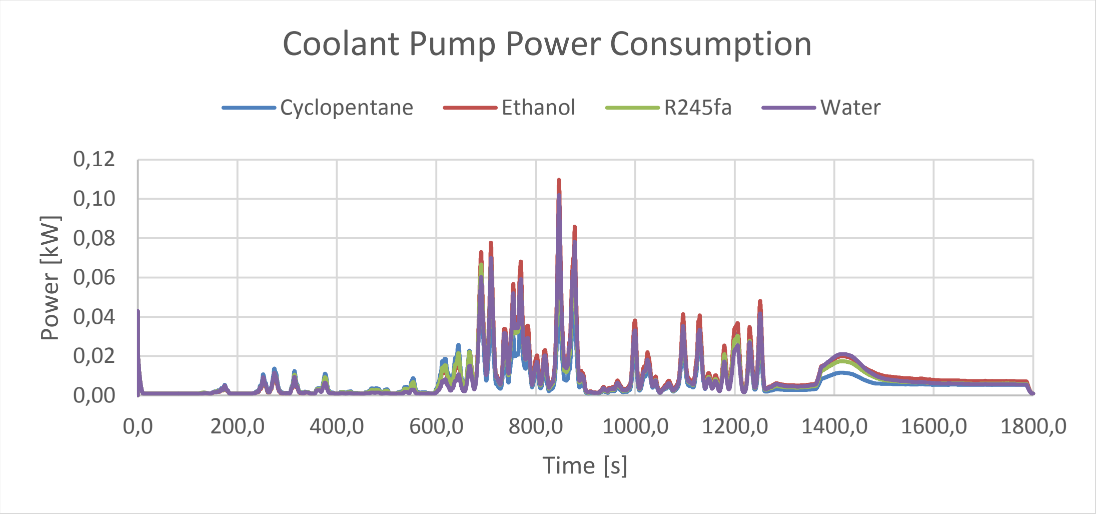

Figure 3.32 : Coolant pump power consumption in transient cycle.

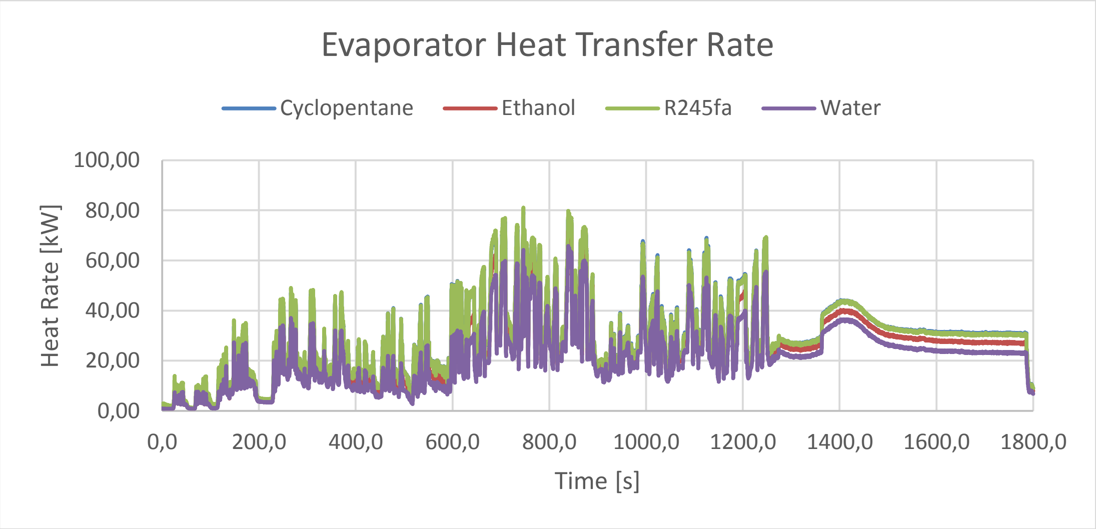

Figure 3.33 : Evaporator heat transfer rate in transient cycle.

Water has the lowest cycle average condenser heat transfer rate due to the lowest evaporator heat rate (Figure 3.34).

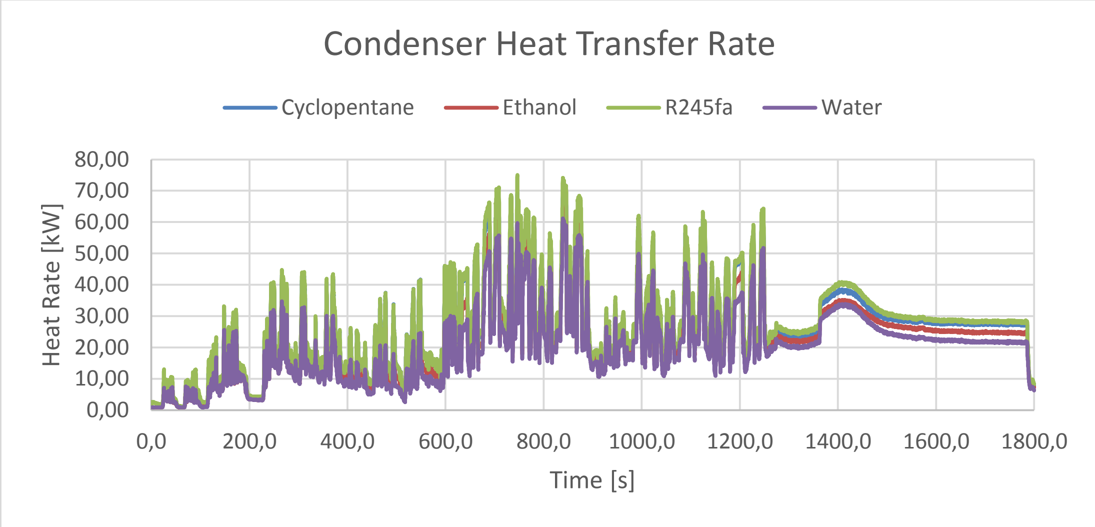

Figure 3.34 : Condenser heat transfer rate in transient cycle.

3.2.5 Sensitivity analysis with REFPROP results

Sensitivity analysis is carried out with transient REFPROP simulation results.

In the following graph, fuel economy benefit is plotted against cycle average evaporation temperature (Figure 3.35). It can be seen that there is a good correlation between fuel economy benefit and cycle average evaporation temperature. This is expected because thermal efficiency of the rankine cycle increases with increasing evaporation temperature.

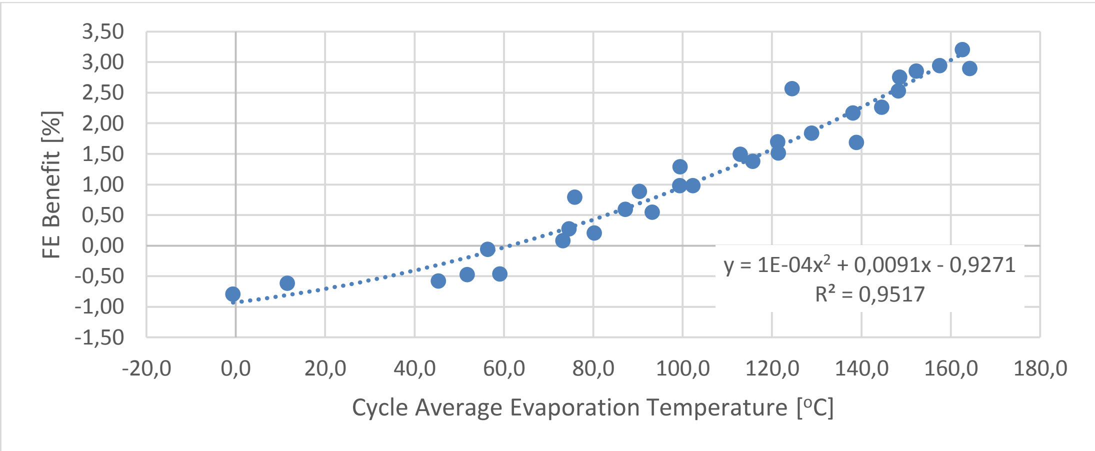

Figure 3.35 : FE benefit vs. cycle average evaporation temperature.

3.3 Simulation Results with COSMO

Simulations are carried out with working fluid properties calculated by COSMOconf software. Simulations are carried out for 129 working fluids. Simulation results show that methanol has the highest fuel economy benefit. Ethanol is the 10th and cyclopentane is the 33th in the ranking. Some of the working fluids have negative fuel economy benefit because it is not possible to condense these working fluids at 20 ^{o}C ambient temperature (Figure 3.36).

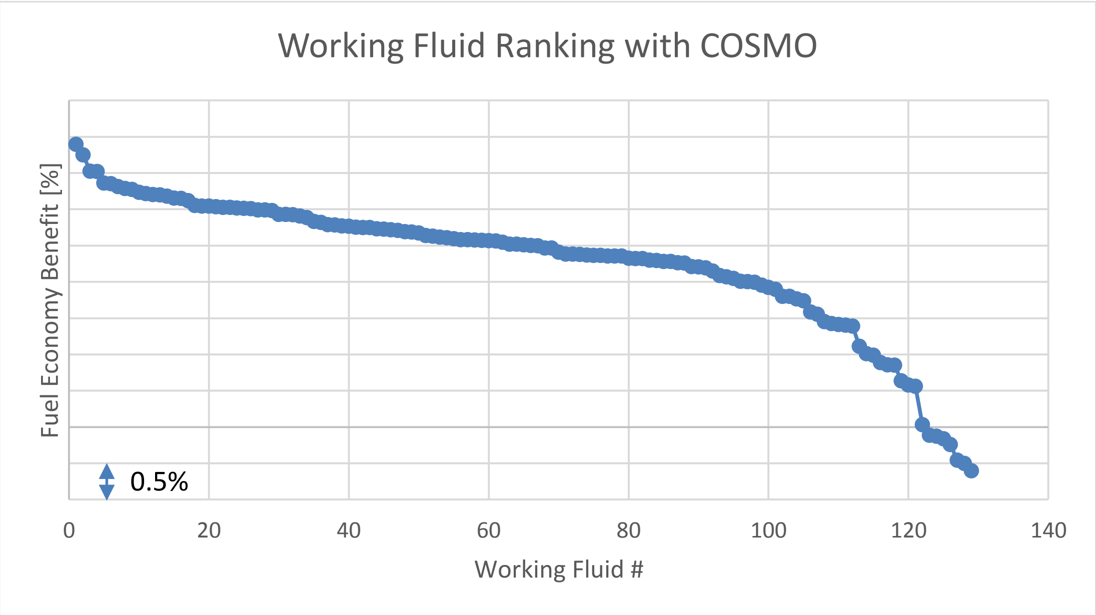

Figure 3.36 : Working fluid ranking with COSMO.

3.4 COSMO vs. REFPROP Simulation Results Comparison

Simulations are carried out with both COSMO and REFPROP softwares for 31 working fluids. There are some differences between COSMO and REFPROP in terms of working fluid rankings. This difference is due to the calculation methodology of working fluid properties with these softwares. The results for fuel economy benefit are compared in the Figure 3.37. There is a good agreement between COSMO and REFPROP results. This result shows that COSMO software is very useful for the assessment of large number of fluids (i.e. thousands of fluids) but working fluid properties should be calculated with REFPROP or tested for a more precise ranking. For example, the ranking results and the results for fuel economy benefit are shown in Table 2.4 for cyclopentane, ethanol, R245fa, and water. Although cyclopentane is the best working fluid among 31 working fluids in

REFPROP ranking, it is 3rd in the COSMO ranking. Fuel economy benefit for cyclopentane is underestimated by 8.5%. Ethanol is the 5th working fluid REFPROP ranking whereas it is the 2nd working fluid in COSMO ranking. Fuel economy benefit for ethanol is overestimated by 19.3% in COSMO calculations. R245fa is the 10th working fluid REFPROP ranking whereas it is the 9th working fluid in COSMO ranking. Fuel economy benefit for R245fa is overestimated by 22.9% in COSMO calculations. Water is the 12th working fluid REFPROP ranking whereas it is the 4th working fluid in COSMO ranking. Fuel economy benefit for water is overestimated by 63.9% in COSMO calculations. These differences are examined in more detail in the following sections.

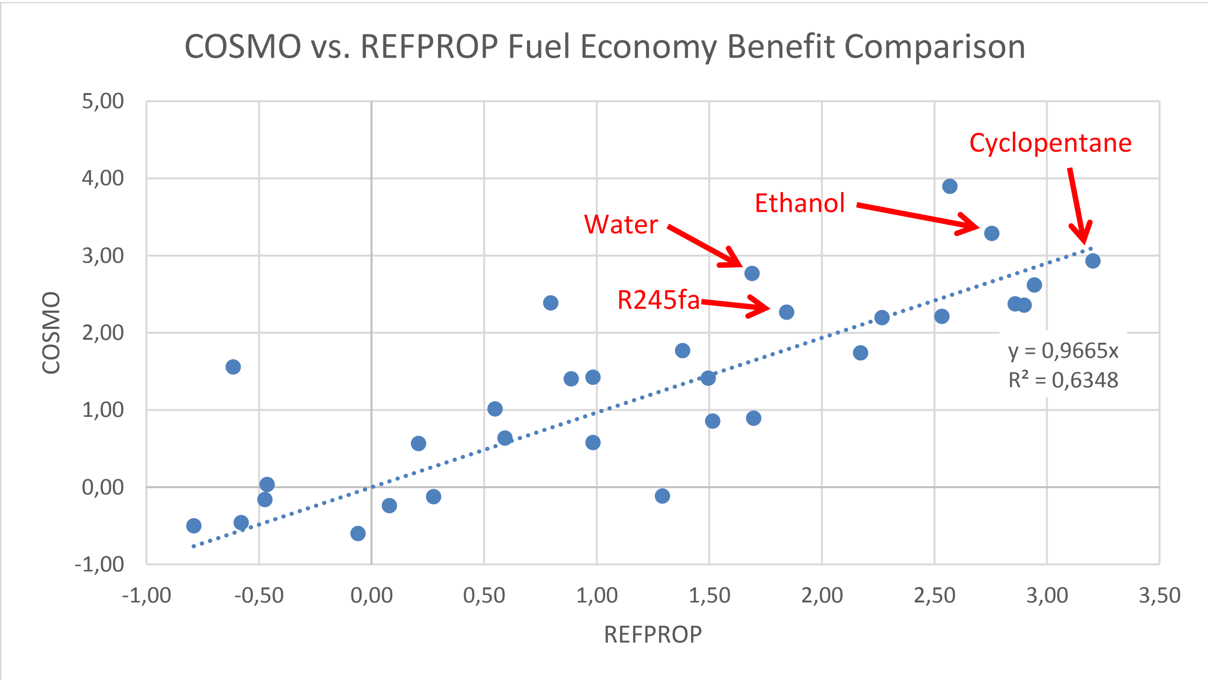

Figure 3.37 : COSMO vs. REFPROP fuel economy benefit comparison.

Table 2.4 : Ranking results comparison.

Parameter	Unit	Cyclop entane	Ethanol	R245fa	Water
Refprop Ranking	#	1	5	10	12
COSMO Ranking	#	3	2	9	4
FE Benefit Difference	%	-8.5	19.3	22.9	63.9

3.4.1 COSMO vs. REFPROP comparison for cyclopentane

Simulation results show that fuel economy benefit and net power is underestimated by 8.5% in COSMO simulations when compared to REFPROP simulations. This is due to 15.8% lower working fluid mass flow rate in COSMO simulations although evaporation temperature is higher by 7.9% (Table 2.5).

Table 2.5 : REFPROP vs. COSMO comparison results for cyclopentane.

Parameter	Unit	REFPROP	COSMO	Percent Difference
FE_Benefit	%	3.20	2.93	-8.5
P_net	kW	2.55	2.33	-8.5
P_exp	kW	3.38	3.15	-6.9
P_ wf_pump	kW	0.21	0.20	-3.3
P_fan	kW	0.61	0.61	-1.4
P_coolant_pump	kW	0.01	0.01	3.0
p_evap	bar	17.6	21.4	22.0
T_evap	ºC	162.6	175.5	7.9
p_cond	bar	1.25	1.24	-0.5
T_cond	ºC	55.9	56.2	0.5
m_wf	kg/s	0.05	0.04	-15.8
Q_wf	L/h	329.22	327.74	-0.5

COSMO evaporation temperature results are in good correlation REFPROP results (Figure 3.38).

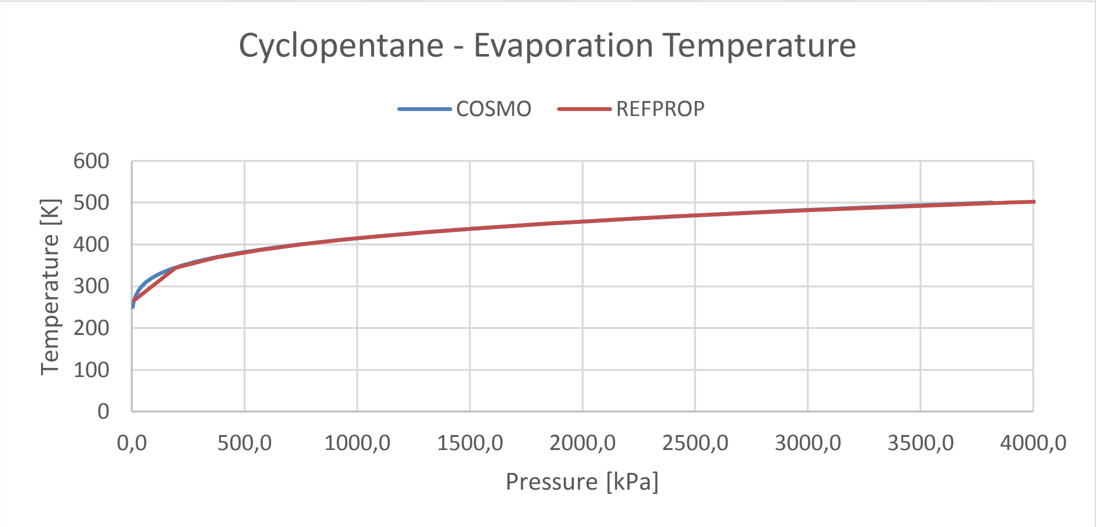

Figure 3.38 : COSMO vs. REFPROP evaporation temperature comparison for cyclopentane.

COSMO enthalpy of vaporization results are also in good correlation with REFPROP results above 1500 kPa. Below 1500 kPa, COSMO overpredicts enthalpy of vaporization (Figure 3.39).

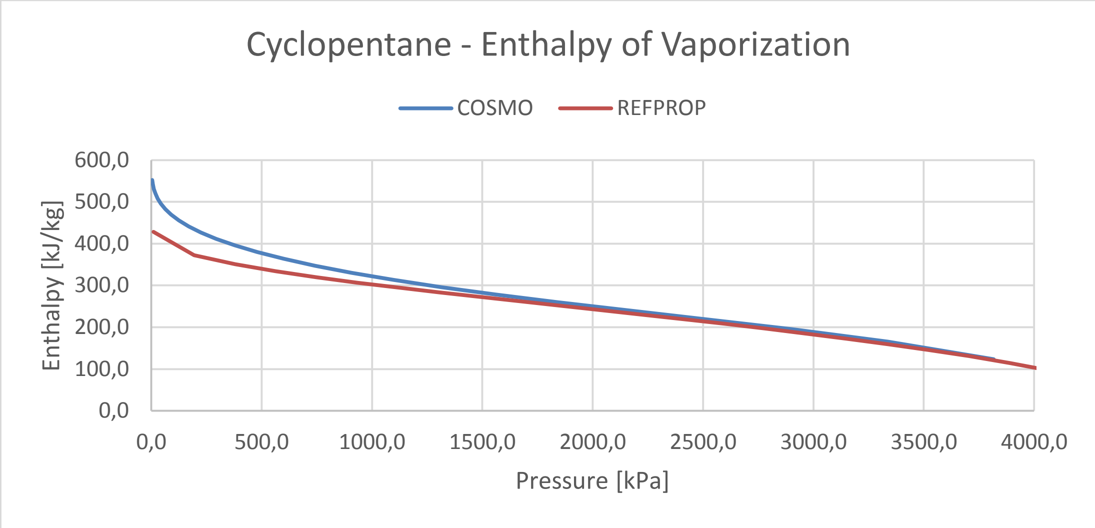

Figure 3.39 : COSMO vs. REFPROP enthalpy of vaporization comparison for cyclopentane.

3.4.2 COSMO vs. REFPROP comparison for ethanol

Simulation results show that the net power of the waster heat recovery system is 19.3% higher in COSMO simulations when compared to REFPROP simulations. This is mainly due to 16.5% higher expander power in COSMO simulations compared to REFPROP simulations. Higher expander power in COSMO is a result of higher mean evaporation temperature as shown in Figure – 11. Cycle average mass flow rate in COSMO is slightly higher due to lower enthalpy of vaporization as shown in Figure – 12. In other words, more mass flow rate is needed for the same evaporator heat rate (Table 2.6).

Table 2.6 : REFPROP vs. COSMO comparison results for ethanol.

Parameter	Unit	REFPROP	COSMO	Percent Difference
FE_Benefit	%	2.75	3.29	19.3
P_net	kW	2.19	2.62	19.3
P_exp	kW	2.41	2.80	16.5
P_ wf_pump	kW	0.07	0.08	12.7
P_fan	kW	0.13	0.10	-24.7
P_coolant_pump	kW	0.01	0.01	-26.3
p_evap	bar	11.4	12.8	12.2
T_evap	ºC	148.6	165.1	11.2
p_cond	bar	0.93	0.92	-1.3
T_cond	ºC	76.1	80.0	5.1
m_wf	kg/s	0.02	0.03	3.9
Q_wf	L/h	141.03	172.16	22.1

COSMO slightly overpredicts ethanol evaporation temperature when compared to REFPROP (Figure 3.40).

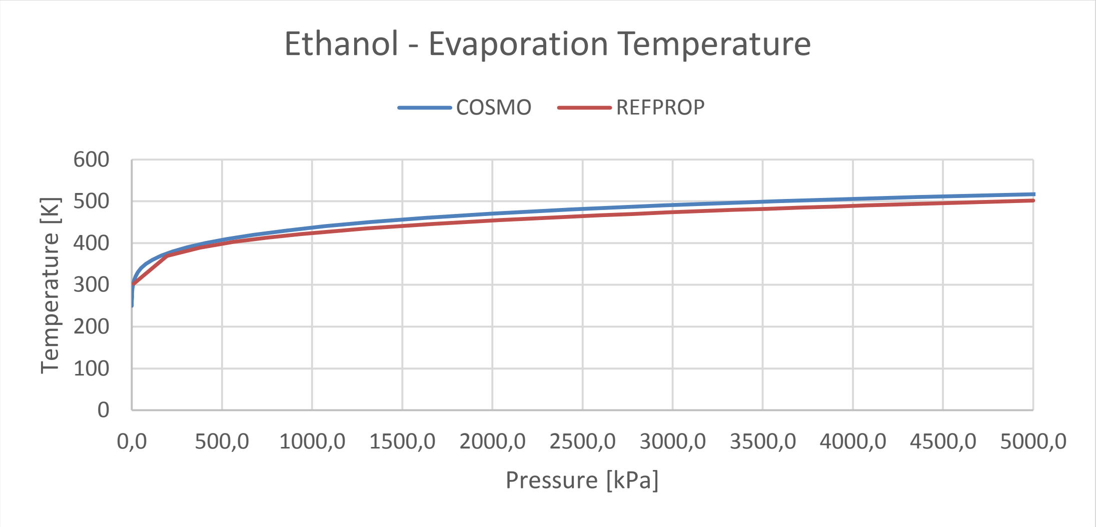

Figure 3.40 : COSMO vs. REFPROP evaporation temperature comparison for ethanol.

COSMO underpredicts ethanol enthalpy of vaporization when compared to REFPROP (Figure 3.41).

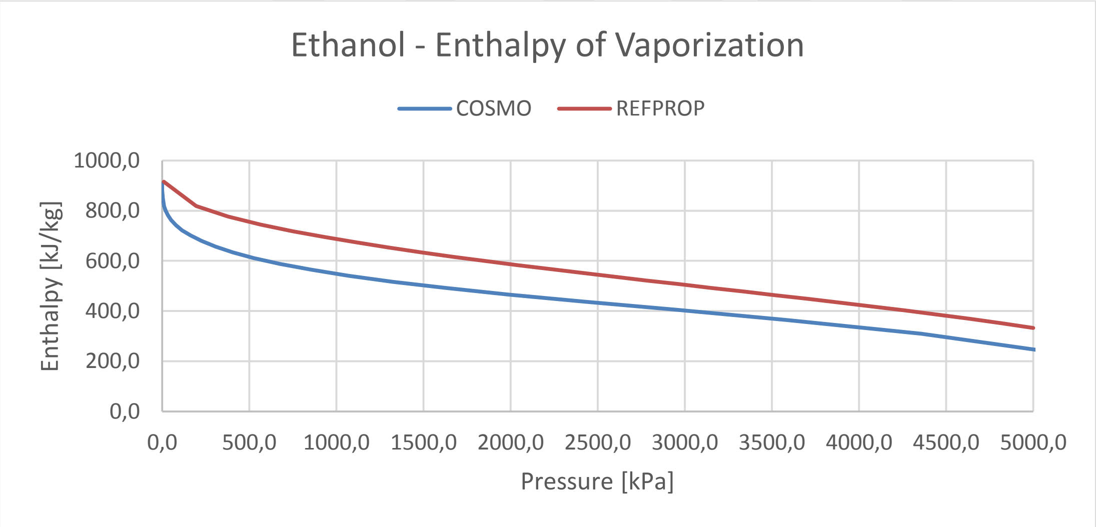

Figure 3.41 : COSMO vs. REFPROP enthalpy of vaporization comparison for ethanol.

3.4.3 COSMO vs. REFPROP comparison for R245fa

Simulation results show that fuel economy benefit and net power generation are 22.9% higher in COSMO simulations when compared to REFPROP simulations. This is due to 24.5% higher evaporation temperature in COSMO simulations (Table 2.7).

Table 2.7 : REFPROP vs. COSMO comparison results for R245fa.

Parameter	Unit	REFPROP	COSMO	Percent Difference
FE_Benefit	%	1.84	2.27	22.9
P_net	kW	1.47	1.80	22.9
P_exp	kW	2.44	2.70	10.5
P_wf_pump	kW	0.30	0.22	-25.2
P_fan	kW	0.67	0.67	-0.2
P_coolant_pump	kW	0.01	0.01	-28.8
p_evap	bar	23.6	21.1	-10.6
T_evap	^{o}C	128.9	160.4	24.5
p_cond	bar	3.95	2.31	-41.5
T_cond	^{o}C	56.2	55.6	-1.0
m_wf	kg/s	0.11	0.08	-24.6
Q_wf	L/h	437.81	423.59	-3.2

COSMO slightly overpredicts R245fa evaporation temperature when compared to REFPROP (Figure 3.42).

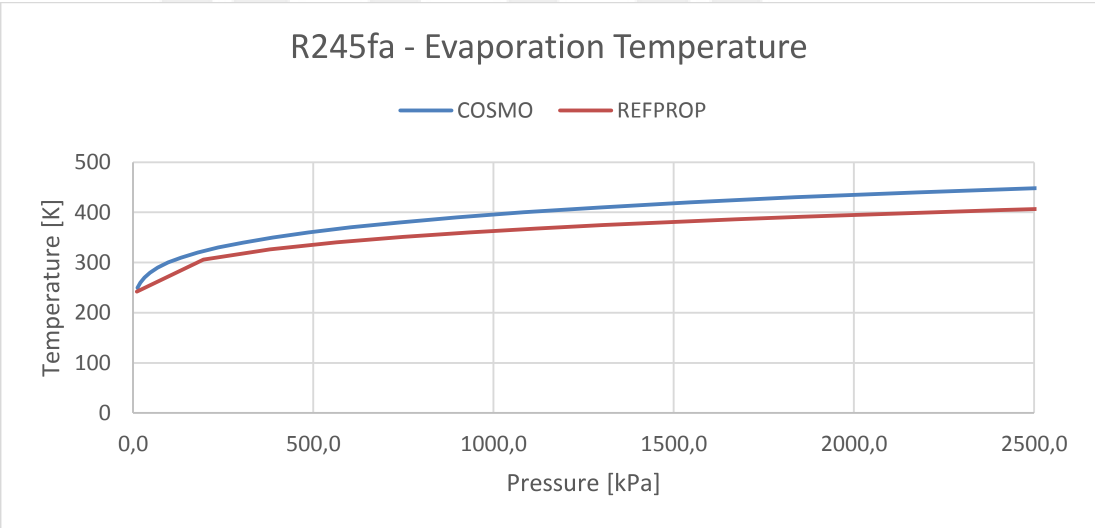

Figure 3.42 : COSMO vs. REFPROP evaporation temperature comparison for R245fa.

COSMO enthalpy of vaporization results are in good correlation with REFPROP results above 1000 kPa. Below 1000 kPa, COSMO overpredicts enthalpy of vaporization for R245fa (Figure 3.43).

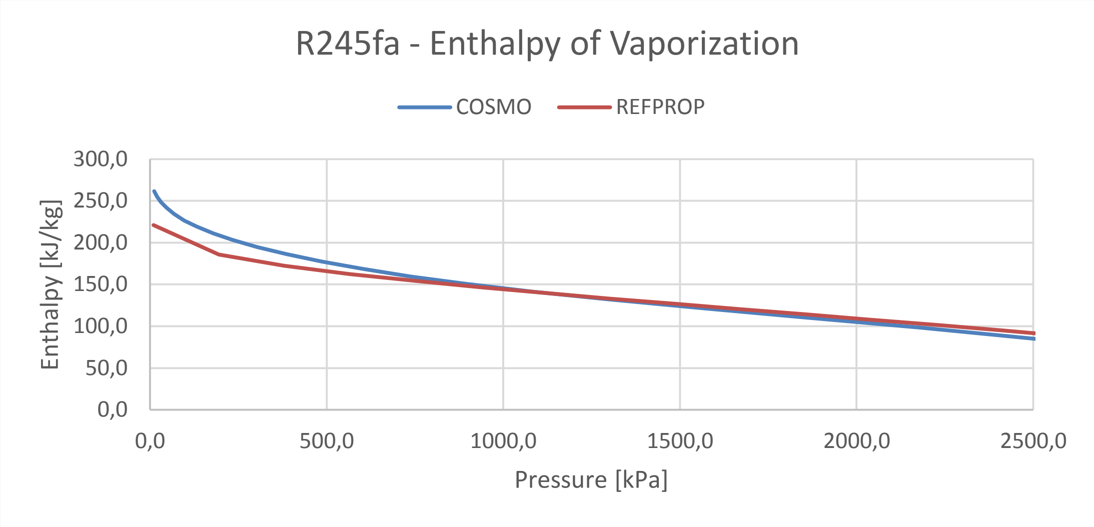

Figure 3.43 : COSMO vs. REFPROP enthalpy of vaporization comparison for R245fa.

3.4.4 COSMO vs. REFPROP comparison for water

Simulation results show that fuel economy benefit and net power generation are 63.9% higher in COSMO simulations when compared to REFPROP simulations. This is due to 24.5% higher evaporation temperature in COSMO simulations (Table 2.8).

Table 2.8 : REFPROP vs. COSMO comparison results for water.

Parameter	Unit	REFPROP	COSMO	Percent Difference
FE_Benefit	%	1.69	2.77	63.9
P_net	kW	1.34	2.20	63.9
P_exp	kW	1.42	2.32	63.7
P_ wf_pump	kW	0.01	0.06	1037.2
P_fan	kW	0.06	0.05	-14.3
P_coolant_pump	kW	0.01	0.01	-19.0
p_evap	bar	3.8	19.4	410.7
T_evap	ºC	138.9	185.2	33.3
p_cond	bar	0.86	0.84	-1.9
T_cond	ºC	93.2	94.3	1.2
m_wf	kg/s	0.01	0.01	25.1
Q_wf	L/h	35.07	225.53	543.1

COSMO and REFPROP results for water evaporation temperature are in good correlation (Figure 3.44).

Enthalpy of vaporization for water is significantly underpredicted when compared to REFPROP (Figure 3.45).

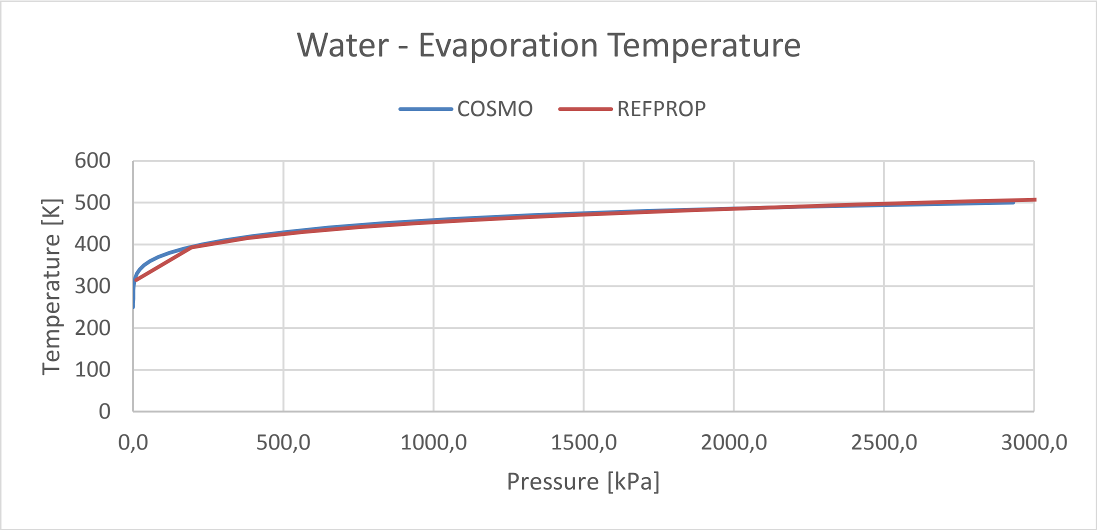

Figure 3.44 : COSMO vs. REFPROP evaporation temperature comparison for water.

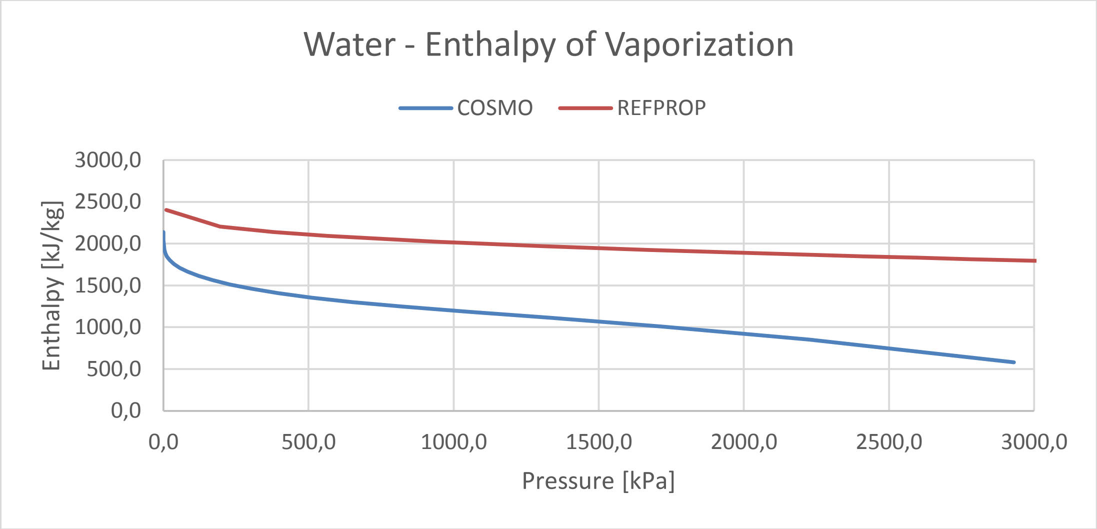

Figure 3.45 : COSMO vs. REFPROP enthalpy of vaporization comparison for water.

4. CONCLUSIONS AND RECOMMENDATIONS

Methanol is found out to be the best working fluid if working fluid properties are calculated by using COSMO software whereas cyclopentane is found out to be the best working fluid with REFPROP software. REFPROP results are more reliable because it calculates the working fluid properties using the most accurate equations available worldwide. Methanol is toxic and flammable but cyclopentane is also flammable but it is non-toxic.

In COSMO simulations, cyclopentane ranking is 31. There are 30 working fluids better than cyclopentane. Properties for some of these are available in REFPROP database. However, most of them are not available in REFPROP database. Hence, it was not possible to carry out simulations for these working fluids with accurate properties data. One of these working fluids could perform better than cyclopentane if accurate properties data were available. As a result, simulations should be carried out for these working fluids with accurate properties data from another source such as testing.

Ethanol is one of the most studied working fluids in literature. It is the 5^{th} working fluid in REFPROP ranking whereas it is the 2^{nd} in COSMO ranking. Ethanol is better than cyclopentane in COSMO ranking but it is worse in REFPROP ranking.

R245fa is another working fluid which is one of the most studied working fluids in literature. It is the 10^{th} working fluid in REFPROP ranking whereas it is the 9^{th} in COSMO ranking. R245fa has worse fuel economy benefit than cyclopentane in both COSMO and REFPROP rankings.

Water is also reported in more detail because it is used in industrial waste heat recovery applications. It is the 12^{th} working fluid in REFPROP ranking whereas it is the 4^{th} in COSMO ranking. Water has also worse fuel economy benefit than cyclopentane in both COSMO and REFPROP rankings.

It is shown that fuel economy benefit increases with increasing evaporation temperature by plotting fuel economy benefit against evaporation temperature in sensitivity analysis section. It is also shown that rankine cycle calculations are aligned with well known phenomena that Rankine cycle efficiency increases with increasing average temperature at which heat is supplied. However, the trend is not strictly monotonic because average temperature at which heat is rejected is not the same for some of the working fluids. The fan control strategy tries to maintain 1.0 bar condensation pressure which is equal to ambient pressure in order to prevent leakage from ambient to the waste heat recovery system. Condensation temperature at 1.0 bar pressure is different for all of the working fluids. For most of the working fluids, it is not possible to maintain target condensation pressure due to very low condensation temperature. For these working fluids, fan operates at maximum speed and condensation temperature becomes almost the same around 60 ^{o}C. If simulations were carried out with a very high cooling capacity, it would be possible to maintain 1.0 bar target condensation pressure for all of working fluids and condensation temperatures would be different for all of working fluids.

It is also shown that working fluids with high condensation pressure have lower fuel economy benefit. It was possible to factor in the effect of condensation pressure by integrating a cooling system model in working fluid ranking simulations.

In steady state T-s diagrams, it is shown that working fluid mass flow rate needs to be higher when operation area is small. In steady state T-q diagrams, it is shown that evaporation temperature becomes higher when heat capacity rate is higher. When heat capacity rate is higher, working fluid temperature increase is lower with the same heat addition. As a result, evaporation temperature is limited at a higher point due to pinch point.

Transient simulation results show that fan speed controller successfully maintains target condensation pressure or it operates fan at maximum when it is not possible to maintain target condensation pressure. It is also shon that evaporation pressure and evaporation temperature is limited successfully according to design limits such as critical temperature, critical pressure, structural limits, etc.

Evaporation temperature and enthalpy of vaporization predicted by COSMO and REFPROP softwares are compared for cyclopentane, ethanol, R245fa, and water. It is shown that COSMO predictions are very accurate in some cases. On the other hand, COSMO software is error prone in some of the cases. These errors lead to fuel economy deviations. Most significant reasons in fuel economy benefit deviations are explained for each working fluid.

This thesis concludes that cyclopentane is the best working fluid for the best fuel economy and safety for a long haul truck.

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APPENDICES

APPENDIX A: Rankine Cycle Function Code

```
function [m_coolant_target, T_coolant_in_target, p_evap_out, P_exp,
T_cond_actual, ...
    P_pump, q_cond, h2, dT2, dT23a, dT23b, dT3, T_exh_out_next,
m_wf, Q_wf, q_evap]  = ...
    Rankine(pp_cond, cp_coolant, superheat, subcool,
T_coolant_in_actual, T_cond_target, ...
    h41a, h1, pump_eff, exp_eff, pp_evap, h_exh_in, ...
    h_exh_out, cp_exh, T_exh_out, T_exh_in, ...
    T_evap, h2s, h23a, h23b, h3, h4s, T2, air_flow, fuel_flow,
p_evap_in, rho_liq)

% q: heat rate (kW)
% T: temperature (C)
% P: power (kW)
% p: pressure (bar)
% h: enthalpy (kJ/kg)
% cp: specific heat (kJ/kg-K)
% m: mass flow rate (kg/s)
% superheat: evaporator superheat (delta K)
% subcool: condenser subcool (delta K)
% pp: pinch point temperature difference (delta K)

m_exh = (air_flow + fuel_flow)/3600;                            %
exhaust mass flow rate
q_evap = m_exh*(h_exh_in - h_exh_out);                          %
evaporator heat transfer rate
h2 = (h2s - h1)/pump_eff+h1;                                    %
enthalpy after pump
m_wf = q_evap/(h3-h2);                                          %
working fluid mass flow rate
h4 = h3 - exp_eff*(h3-h4s);                                     %
enthalpy at expander outlet
P_exp = m_wf * (h3-h4);                                         %
expander power
P_pump = m_wf * (h2-h1);                                        % pump
power
q_cond = m_wf * (h4-h1);                                        %
condenser heat rejection
T3 = T_evap + superheat;                                        %
temperature at expander inlet
T_exh_23a = T_exh_out + (m_wf*(h23a-h2))/(m_exh*cp_exh);        %
exhaust temperature at 23a
T_exh_23b = T_exh_23a + (m_wf*(h23b-h23a))/(m_exh*cp_exh);      %
exhaust temperature at 23b
dT2 = T_exh_out - T2;                                           %
temperature difference at 2
dT23a = T_exh_23a - T_evap;                                     %
temperature difference at 23a
```

```
dT23b = T_exh_23b - T_evap;                                    %
temperature difference at 23b
dT3 = T_exh_in - T3;                                           %
temperature difference at 3
min_dT = min([dT23a dT23b dT3]);                               %
evaporator minimum pinch point temperature difference
p_evap_out = p_evap_in + 0.1*(min_dT - pp_evap);               % next
step evaporation pressure
T_exh_out_next = T_exh_out - 0.1*(dT2 - 4*pp_evap);            % next
evaporator gas outlet temperature

T_cond_actual = T_coolant_in_actual + pp_cond + subcool;
% actual condensation temperature
T_41a_coolant_target = T_cond_target - pp_cond;
% target coolant temperature at 41a
T_coolant_in_target = T_cond_target - subcool - pp_cond;
% target condenser coolant inlet temperature
m_coolant_target=(m_wf*(h41a-h1))/(cp_coolant*(T_41a_coolant_target-
T_coolant_in_target)); % target coolant mass flow rate

Q_wf = (m_wf/max(rho_liq,1))*3.6e6;
% liquid phase volume flow rate (L/h)
```

APPENDIX B: *.m file Code for Working Fluid Iterations with COSMO

```
%% Import data from text file.
% Script for importing data from the following text file:
%
%    C:\Users\msimsek5\Desktop\Delete\script_size_deneme\177.tab
%
% To extend the code to different selected data or a different text
file,
% generate a function instead of a script.

% Auto-generated by MATLAB on 2016/11/15 17:44:07

%% Iterate for different working fluids

clc

% Failed working fluids due to Matlab

% wf = [527 1031 6337 7853 68041 17789749]
% wf_name = {'propionaldehyde','1-
propanol','chloroethane','ALLYLAMINE','1,3-
DIFLUOROPROPANE','Difluoromethanol'}

wf = [177 180 222 241 702 712 878 887 962 3776 6323 6329 6332 6333
6334 6335 6338 6341 6344 6351 6361 6366 ...
    6370 6382 6389 6409 7844 7850 7860 7861 7865 8024 8029 8255 9253
9385 9773 9871 10899 11199 11203 11641 ...
    11643 12223 12722 12983 15373 15442 15586 33239 61108 62407
62695 67754 67895 67898 68030 79058 ...
    93560 123139 136259 141483 150183 164579 542706 588440 638186
643833 2736499 2776731 2779024 2782256 ...
    3494771 5284364 5287573 5326315 5370463 5372670 5463043 5463331
5709018 5709597 9942119 10154032 ...
```

```
    10486802 10931411 10953482 11996923 17904871 17911648 17992575
18532994 18769290 ...
    18960304 19350069 19851878 19860156 20271514 20637462 20762084
21439578 21572609 21614694 ...
    21731211 23233663 23233664 23261771 45933721 54438463 55299800
57449531 59908015 71359705 ...
    6345 6324 6368 6388 9868 5708720 17822 9633 69624 79009 6428
6429 6430 6431 67940 8263];

wf_name =
{'Acetaldehyde','Acetone','Ammonia','Benzene','Ethanol','Formaldehyd
e','Methanethiol','Methanol','Water',...

'Isopropanol','Bromomethane','METHYLAMINE','Bromoethane','Bromochlor
omethane','Propane','Propyne','Chloroethylene',...
    'Ethanamine','DICHLOROMETHANE','CYCLOPROPANE','2-
CHLOROPROPANE','Vinylidene Chloride','Dichlorofluoromethane',...
    'DIBROMODIFLUOROMETHANE','Trichlorofluoromethane','2,2,2-
TRIFLUOROETHANOL','1-BUTENE','ALLYL CHLORIDE',...
    'GLYOXAL','Methoxyethene','METHYL FORMATE','Vinyl
Ether','FURAN','Isobutene','CYCLOPENTANE',...
    '2,2-DICHLORO-1,1,1-TRIFLUOROETHANE','2,2,2-
Trifluoroethylamine','1,1,1-TRIFLUOROACETONE','1-CHLOROPROPANE',...
    'Ethenol','2-Chloropropene','VINYL
BROMIDE','CHLOROFLUOROMETHANE','1,2-DIFLUOROETHANE',...
    '1,1,1,3,3,3-Hexafluoropropane','1-Chloro-2-fluoroethane','1-
Chloro-1-fluoroethane',...
    '1,2-DICHLORO-1,1-DIFLUOROETHANE','1,1-DICHLORO-1-
FLUOROETHANE','1,1-DICHLORO-1,2-DIFLUOROETHANE',...
    'Bromofluoromethane','Bromodifluoromethane','trans-2-Butene','2-
Bromo-1,1-difluoroethene','2,2-Difluoropropane',...
    '2-Bromo-1,1,1-trifluoroethane','1,1,1,3,3-
Pentafluoropropane','Bromochlorofluoromethane',...
    'Chlorodifluoroacetaldehyde','Methanimine','1-Bromo-1,1-
difluoroethane','Propen-2-ol','1-CHLORO-1-FLUOROPROPANE',...
    '1-Chloro-1,2-difluoroethane','Trifluoromethanamine','1-bromo-
1,2-difluoroethene','TRANS-1,2-DICHLOROETHYLENE',...
    'CIS-1,2-DICHLOROETHYLENE','2-Chloro-1,1-
difluoroethane','2,3,3,3-tetrafluoropropene',...
    '3,3,3-trifluoro-2-oxopropanal','1-Bromo-1-fluoroethylene','1,1-
difluoroacetone','1-Chloropropene',...
    'cis-2-Butene','1-Chloro-propene','1,2-Dichloro-1-
fluoroethylene','1-bromo-1,2-difluoroethene',...
    'Ethene, 1-bromo-2-fluoro-, (Z)-','(Z)-1-Propenol','2730-43-
0','(E/Z)-1-Bromo-2-fluoroethylene',...
    '2,2-difluoroacetaldehyde','1,1,3,3-tetrafluoropropane','1,1,2-
trifluoropropane',...
    'Ethene, 1,1-dichloro-2-fluoro-','1-fluoroethanimine','Ethane,
(difluoromethoxy)-',...
    'PROPANAL, 2,2-DIFLUORO-','[CHLORO(DIFLUORO)METHYL] FORMATE','1-
FLUORO-1-METHOXYETHENE','SCHEMBL24745',...
    'Methanol, chlorofluoro-','1,2-difluoropropane','ETHANOL,
1,2,2,2-TETRAFLUORO-','3-CHLORO-3-FLUOROPROP-1-ENE',...
    'N-Methyltrifluoromethanamine','1,3-Dioxole, 2,2,4-trifluoro-
','1-FLUORO-1-(FLUOROMETHOXY)ETHENE',...
    'Ethane, 1-fluoro-1-methoxy-','2,4,5-TRIFLUORO-1,3-
OXAZOLE','1,2-Dichloro-1-fluoroethylene','2,4-Difluorofuran',...
    '1-Propene, 2-bromo-1-fluoro-, (E)-','(E)-1-Chloro-2-fluoro-1-
propene','(Z)-1-Chloro-2-fluoroprop-1-ene',...
    '1-BROMO-1,1,2-TRIFLUOROETHANE','3-Chloro-1,1-difluoroprop-1-
ene','CHLORO-DIFLUORO-METHOXYMETHANE',...
```

```
    'METHANAMINE, N-(DIFLUOROMETHYL)-1,1,1-TRIFLUORO-','1-
Fluoroethen-1-ol',...
    'N-METHYLMETHANIMIDOYL FLUORIDE','Methanimidoyl Fluoride',...

'R32','ETHANE','R152a','R142b','R143a','R1234ze','R124','R125','R245
ca','R236ea','R113','R114','R115','R116','R227ea','RC318'};

wf_size = size(wf);
disp(strcat('Number of working fluids:',num2str(wf_size(2))));

s1 = 'F:\Active Projects\WHR\GT-SUITE Files\COSMOlogic_Coupling\';
s3 = '.tab';

c = fix(clock); % date & time
new_sheet = strcat(num2str(c(1)),'-',num2str(c(2)),'-
',num2str(c(3)),'_',num2str(c(4)),'-',num2str(c(5)));

    xlswrite('Matlab_Simulation_Results.xlsx',{'CID
(PubChem)'},new_sheet,'A1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'Name
(PubChem)'},new_sheet,'B1');

P_net_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_net_mean'},new_sheet,'
C1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'C2');
Brake_Power_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Brake_Power_mean'},new_s
heet,'D1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'D2');
FE_Benefit = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'FE_Benefit'},new_sheet,'
E1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'%'},new_sheet,'E2');

P_exp_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_min'},new_sheet,'F
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'F2');
P_exp_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_max'},new_sheet,'G
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'G2');
P_exp_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_mean'},new_sheet,'
H1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'H2');

P_pump_min = ones(1,wf_size(2));
```

```
xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_min'},new_sheet,'
I1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'I2');
P_pump_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_max'},new_sheet,'
J1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'J2');
P_pump_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_mean'},new_sheet,
'K1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'K2');

P_fan_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_min'},new_sheet,'L
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'L2');
P_fan_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_max'},new_sheet,'M
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'M2');
P_fan_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_mean'},new_sheet,'
N1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'N2');

P_coolant_pump_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_min'},new
_sheet,'O1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'O2');
P_coolant_pump_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_max'},new
_sheet,'P1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'P2');
P_coolant_pump_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_mean'},ne
w_sheet,'Q1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'Q2');

p_evap_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_min'},new_sheet,'
R1');
```

```
xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'R2');
p_evap_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_max'},new_sheet,'
S1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'S2');
p_evap_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_mean'},new_sheet,
'T1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'T2');

T_evap_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_min'},new_sheet,'
U1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'U2');
T_evap_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_max'},new_sheet,'
V1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'V2');
T_evap_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_mean'},new_sheet,
'W1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'W2');

p_cond_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_min'},new_sheet,'
X1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'X2');
p_cond_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_max'},new_sheet,'
Y1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'Y2');
p_cond_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_mean'},new_sheet,
'Z1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'Z2');

T_cond_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_min'},new_sheet,'
AA1');

xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AA2');
T_cond_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_max'},new_sheet,'
AB1');
```

```
xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AB2');
T_cond_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_mean'},new_sheet,
'AC1');

xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AC2');

m_wf_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_min'},new_sheet,'AD
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AD2');
m_wf_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_max'},new_sheet,'AE
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AE2');
m_wf_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_mean'},new_sheet,'A
F1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AF2');

Q_wf_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_min'},new_sheet,'AG
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AG2');
Q_wf_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_max'},new_sheet,'AH
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AH2');
Q_wf_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_mean'},new_sheet,'A
I1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AI2');

% successful_fluids =
fopen('01_successfully_simulated_working_fluids.txt','w');  % list
of successfully simulated fluids

for i = 1:wf_size(2)
    s2 = num2str(wf(i));
    disp(strcat('Fluid #',num2str(i),': ',s2));

    %% Initialize variables.
    %filename = 'F:\Active Projects\WHR\GT-SUITE
Files\COSMOlogic_Coupling\702.tab';
    filename = strcat(s1,s2,s3);
    startRow = 5;
```

```
    %% Read columns of data as strings:
    % For more information, see the TEXTSCAN documentation.
    formatSpec = '%16s%16s%16s%16s%16s%16s%16s%16s%s%[^\n\r]';

    %% Open the text file.
    fileID = fopen(filename,'r');

    %% Read columns of data according to format string.
    % This call is based on the structure of the file used to
generate this
    % code. If an error occurs for a different file, try
regenerating the code
    % from the Import Tool.
    textscan(fileID, '%[^\n\r]', startRow-1, 'ReturnOnError',
false);
    dataArray = textscan(fileID, formatSpec, 'Delimiter', '',
'WhiteSpace', '', 'ReturnOnError', false);

    %% Close the text file.
    fclose(fileID);

    %% Convert the contents of columns containing numeric strings to
numbers.
    % Replace non-numeric strings with NaN.
    raw = repmat({''},length(dataArray{1}),length(dataArray));
    for col=1:length(dataArray)-1
        raw(1:length(dataArray{col}),col) = dataArray{col};
    end
    numericData = NaN(size(dataArray{1},1),size(dataArray,2));

    for col=[1,2,3,4,5,6,7,8,9,10]
        % Converts strings in the input cell array to numbers.
Replaced non-numeric
        % strings with NaN.
        rawData = dataArray{col};
        for row=1:size(rawData, 1);
            % Create a regular expression to detect and remove non-
numeric prefixes and
            % suffixes.
            regexstr = '(?<prefix>.*?)(?<numbers>([-
]*(\d+[\,]*)+[\.]{0,1}\d*[eEdD]{0,1}[-+]*\d*[i]{0,1})|([-
]*(\d+[\,]*)*[\.]{1,1}\d+[eEdD]{0,1}[-
+]*\d*[i]{0,1}))(?<suffix>.*)';
            try
                result = regexp(rawData{row}, regexstr, 'names');
                numbers = result.numbers;

                % Detected commas in non-thousand locations.
                invalidThousandsSeparator = false;
                if any(numbers==',');
                    thousandsRegExp = '^\d+?(\,\d{3})*\.{0,1}\d*$';
                    if isempty(regexp(thousandsRegExp, ',',
'once'));
                        numbers = NaN;
                        invalidThousandsSeparator = true;
                    end
                end
                % Convert numeric strings to numbers.
                if ~invalidThousandsSeparator;
```

```
                    numbers = textscan(strrep(numbers, ',', ''),
'%f');
                    numericData(row, col) = numbers{1};
                    raw{row, col} = numbers{1};
                end
            catch me
            end
        end
    end

    %% Replace non-numeric cells with 0.0
    R = cellfun(@(x) (~isnumeric(x) && ~islogical(x)) ||
isnan(x),raw); % Find non-numeric cells
    raw(R) = {0.0}; % Replace non-numeric cells

    %% Allocate imported array to column variable names
    Temperature = cell2mat(raw(:, 1));
    Pressure = cell2mat(raw(:, 2));
    Phase = cell2mat(raw(:, 3));
    EnthalpyLiq = cell2mat(raw(:, 4));
    EnthalpyVap = cell2mat(raw(:, 5));
    EntropyLiq = cell2mat(raw(:, 6));
    EntropyVap = cell2mat(raw(:, 7));
    DensityLiq = cell2mat(raw(:, 8));
    DensityVap = cell2mat(raw(:, 9));
    Warning = cell2mat(raw(:, 10));

    %% Lookup calculations
    tab_file_size=size(numericData);
    number_of_rows = tab_file_size(1);
    sat_end = number_of_rows - 5;
    number_of_sat_rows = floor(Temperature(number_of_rows)/10)-25;
    sat_start = sat_end - (number_of_sat_rows - 1);
    phase_end = sat_start - 5;

    T_min=min(Temperature(1:phase_end));
T_max=max(Temperature(1:phase_end));
    p_min=min(Pressure(1:phase_end));
p_max=max(Pressure(1:phase_end));
    h_liq_min=min(EnthalpyLiq(1:phase_end));
h_liq_max=max(EnthalpyLiq(1:phase_end));
    h_vap_min=min(EnthalpyVap(1:phase_end));
h_vap_max=max(EnthalpyVap(1:phase_end));
    s_liq_min=min(EntropyLiq(1:phase_end));
s_liq_max=max(EntropyLiq(1:phase_end));
    s_vap_min=min(EntropyVap(1:phase_end));
s_vap_max=max(EntropyVap(1:phase_end));

    [p_ph_T_liq,h_ph_T_liq]=meshgrid(p_min:25:p_max,
h_liq_min:0.1:h_liq_max);

ph_T_liq=griddata(Pressure(1:phase_end),EnthalpyLiq(1:phase_end),Tem
perature(1:phase_end),p_ph_T_liq,h_ph_T_liq);
    ph_T_liq(isnan(ph_T_liq))=0;

    [T_Tp_h_liq,p_Tp_h_liq]=meshgrid(T_min:10:T_max,
p_min:25:p_max);

Tp_h_liq=griddata(Temperature(1:phase_end),Pressure(1:phase_end),Ent
halpyLiq(1:phase_end),T_Tp_h_liq,p_Tp_h_liq);
```

```
    Tp_h_liq(isnan(Tp_h_liq))=0;

    [T_Tp_s_liq,p_Tp_s_liq]=meshgrid(T_min:10:T_max,
p_min:25:p_max);

Tp_s_liq=griddata(Temperature(1:phase_end),Pressure(1:phase_end),Ent
ropyLiq(1:phase_end),T_Tp_s_liq,p_Tp_s_liq);
    Tp_s_liq(isnan(Tp_s_liq))=0;

    [p_ps_h_liq,s_ps_h_liq]=meshgrid(p_min:25:p_max,
s_liq_min:0.02:s_liq_max);

ps_h_liq=griddata(Pressure(1:phase_end),EntropyLiq(1:phase_end),Enth
alpyLiq(1:phase_end),p_ps_h_liq,s_ps_h_liq);
    ps_h_liq(isnan(ps_h_liq))=0;

    [T_Tp_h_vap,p_Tp_h_vap]=meshgrid(T_min:10:T_max,
p_min:25:p_max);

Tp_h_vap=griddata(Temperature(1:phase_end),Pressure(1:phase_end),Ent
halpyVap(1:phase_end),T_Tp_h_vap,p_Tp_h_vap);
    Tp_h_vap(isnan(Tp_h_vap))=0;

    [T_Tp_s_vap,p_Tp_s_vap]=meshgrid(T_min:10:T_max,
p_min:25:p_max);

Tp_s_vap=griddata(Temperature(1:phase_end),Pressure(1:phase_end),Ent
ropyVap(1:phase_end),T_Tp_s_vap,p_Tp_s_vap);
    Tp_s_vap(isnan(Tp_s_vap))=0;

    [p_ps_h_vap,s_ps_h_vap]=meshgrid(p_min:25:p_max,
s_vap_min:0.02:s_vap_max);

ps_h_vap=griddata(Pressure(1:phase_end),EntropyVap(1:phase_end),Enth
alpyVap(1:phase_end),p_ps_h_vap,s_ps_h_vap);
    ps_h_vap(isnan(ps_h_vap))=0;

    %% Clear temporary variables
    %clearvars filename startRow formatSpec fileID dataArray ans raw
col numericData rawData row regexstr result numbers
invalidThousandsSeparator thousandsRegExp me R;

    %% Run Simuink model
    simOut =
sim('COSMOlogic_Coupling_R2012b_v5','SimulationMode','normal','AbsTo
l','1e-5',...
                'SaveState','on','StateSaveName','xout',...

'SaveOutput','on','OutputSaveName','yout','SaveFormat',
'StructureWithTime',...
                'SignalLogging','on','SignalLoggingName','logsout');
    %outputs = simOut.get('yout');
    %simOutVars = simOut.who;
    logsout = simOut.get('logsout');

xlswrite('Matlab_Simulation_Results.xlsx',wf(i),new_sheet,strcat('A'
,num2str(i+2)));

xlswrite('Matlab_Simulation_Results.xlsx',wf_name(i),new_sheet,strca
t('B',num2str(i+2)));
```

```
    P_net = logsout.get('P_net');
    P_net_mean(i) = mean(P_net.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_net_mean(i),new_sheet,st
rcat('C',num2str(i+2)));

    Brake_Power = logsout.get('Brake_Power');
    Brake_Power_mean(i) = mean(Brake_Power.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Brake_Power_mean(i),new_sh
eet,strcat('D',num2str(i+2)));

    FE_Benefit(i) = (P_net_mean(i)/Brake_Power_mean(i))*100;

xlswrite('Matlab_Simulation_Results.xlsx',FE_Benefit(i),new_sheet,st
rcat('E',num2str(i+2)));

    P_exp = logsout.get('P_exp');
    P_exp_min(i) = min(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_min(i),new_sheet,str
cat('F',num2str(i+2)));
    P_exp_max(i) = max(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_max(i),new_sheet,str
cat('G',num2str(i+2)));
    P_exp_mean(i) = mean(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_mean(i),new_sheet,st
rcat('H',num2str(i+2)));

    P_pump = logsout.get('P_pump');
    P_pump_min(i) = min(P_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_pump_min(i),new_sheet,st
rcat('I',num2str(i+2)));
    P_pump_max(i) = max(P_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_pump_max(i),new_sheet,st
rcat('J',num2str(i+2)));
    P_pump_mean(i) = mean(P_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_pump_mean(i),new_sheet,s
trcat('K',num2str(i+2)));

    P_fan = logsout.get('P_fan');
    P_fan_min(i) = min(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_min(i),new_sheet,str
cat('L',num2str(i+2)));
    P_fan_max(i) = max(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_max(i),new_sheet,str
cat('M',num2str(i+2)));
    P_fan_mean(i) = mean(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_mean(i),new_sheet,st
rcat('N',num2str(i+2)));
```

```
    P_coolant_pump = logsout.get('P_coolant_pump');
    P_coolant_pump_min(i) = min(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_min(i),new_
sheet,strcat('O',num2str(i+2)));
    P_coolant_pump_max(i) = max(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_max(i),new_
sheet,strcat('P',num2str(i+2)));
    P_coolant_pump_mean(i) = mean(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_mean(i),new
_sheet,strcat('Q',num2str(i+2)));

    p_evap = logsout.get('p_evap_in');
    p_evap_min(i) = min(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_min(i),new_sheet,st
rcat('R',num2str(i+2)));
    p_evap_max(i) = max(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_max(i),new_sheet,st
rcat('S',num2str(i+2)));
    p_evap_mean(i) = mean(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_mean(i),new_sheet,s
trcat('T',num2str(i+2)));

    T_evap = logsout.get('T_evap');
    T_evap_min(i) = min(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_min(i),new_sheet,st
rcat('U',num2str(i+2)));
    T_evap_max(i) = max(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_max(i),new_sheet,st
rcat('V',num2str(i+2)));
    T_evap_mean(i) = mean(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_mean(i),new_sheet,s
trcat('W',num2str(i+2)));

    p_cond = logsout.get('p_cond_actual');
    p_cond_min(i) = min(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_min(i),new_sheet,st
rcat('X',num2str(i+2)));
    p_cond_max(i) = max(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_max(i),new_sheet,st
rcat('Y',num2str(i+2)));
    p_cond_mean(i) = mean(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_mean(i),new_sheet,s
trcat('Z',num2str(i+2)));

    T_cond = logsout.get('T_cond_actual');
    T_cond_min(i) = min(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_min(i),new_sheet,st
rcat('AA',num2str(i+2)));
```

```
    T_cond_max(i) = max(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_max(i),new_sheet,st
rcat('AB',num2str(i+2)));
    T_cond_mean(i) = mean(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_mean(i),new_sheet,s
trcat('AC',num2str(i+2)));

    m_wf = logsout.get('m_wf');
    m_wf_min(i) = min(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_min(i),new_sheet,strc
at('AD',num2str(i+2)));
    m_wf_max(i) = max(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_max(i),new_sheet,strc
at('AE',num2str(i+2)));
    m_wf_mean(i) = mean(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_mean(i),new_sheet,str
cat('AF',num2str(i+2)));

    Q_wf = logsout.get('Q_wf');
    Q_wf_min(i) = min(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_min(i),new_sheet,strc
at('AG',num2str(i+2)));
    Q_wf_max(i) = max(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_max(i),new_sheet,strc
at('AH',num2str(i+2)));
    Q_wf_mean(i) = mean(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_mean(i),new_sheet,str
cat('AI',num2str(i+2)));

    %plot(P_net.Values);

    %% Clear variables
    %clearvars -except wf wf_size s1 s3 P_net_mean Brake_Power_mean
FE_Benefit;

    %% Print successfully simulated working fluids
    %fprintf(successful_fluids,'%d\r\n',wf(i));

end
```

APPENDIX C: *.m file Code for Working Fluid Iterations with REFPROP

```
clc

wf = [222 7843 7844 8078 9253 6351 15600 6324 ...
    702 6325 8900 8058 6360 297 887 ...
    6334 8252 6389 449449 5289250 6393 6372 6373 6345 11638 6428
6429 6430 6431 ...
```

```
    9385 17822 9633 13129 15586 6388 9868 6368 67940 79009 12722
69624 68030 ...
    5709018 2776731 5708720 8263 1140 962];

wf_name =
{'Ammonia','Butane','Butene','CycloHexane','CycloPentane','CycloProp
ane','Decane','Ethane',...

'Ethanol','Ethylene','Heptane','Hexane','Isobutane','Methane','Metha
nol',...

'Propane','Propylene','R11','R12','R13','R14','R22','R23','R32','R41
','R113','R114','R115','R116',...

'R123','R124','R125','R134a','R141b','R142b','R143a','R152a','R227ea
','R236ea','R236fa','R245ca','R245fa',...
    'R1233ZD','R1234YF','R1234ZE','RC318','Toluene','Water'};

wf_size = size(wf);
disp(strcat('Number of working fluids:',num2str(wf_size(2))));

c = fix(clock); % date & time
new_sheet = strcat(num2str(c(1)),'-',num2str(c(2)),'-
',num2str(c(3)),'_',num2str(c(4)),'-',num2str(c(5)));

    xlswrite('Matlab_Simulation_Results.xlsx',{'CID
(PubChem)'},new_sheet,'A1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'Name
(PubChem)'},new_sheet,'B1');

P_net_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_net_mean'},new_sheet,'
C1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'C2');
Brake_Power_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Brake_Power_mean'},new_s
heet,'D1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'D2');
FE_Benefit = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'FE_Benefit'},new_sheet,'
E1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'%'},new_sheet,'E2');

P_exp_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_min'},new_sheet,'F
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'F2');
P_exp_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_max'},new_sheet,'G
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'G2');
```

```
P_exp_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_exp_mean'},new_sheet,'
H1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'H2');

P_pump_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_min'},new_sheet,'
I1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'I2');
P_pump_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_max'},new_sheet,'
J1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'J2');
P_pump_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_pump_mean'},new_sheet,
'K1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'K2');

P_fan_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_min'},new_sheet,'L
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'L2');
P_fan_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_max'},new_sheet,'M
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'M2');
P_fan_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_fan_mean'},new_sheet,'
N1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'N2');

P_coolant_pump_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_min'},new
_sheet,'O1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'O2');
P_coolant_pump_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_max'},new
_sheet,'P1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'P2');
P_coolant_pump_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'P_coolant_pump_mean'},ne
w_sheet,'Q1');
```

```
xlswrite('Matlab_Simulation_Results.xlsx',{'kW'},new_sheet,'Q2');

p_evap_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_min'},new_sheet,'
R1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'R2');
p_evap_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_max'},new_sheet,'
S1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'S2');
p_evap_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_evap_mean'},new_sheet,
'T1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'T2');

T_evap_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_min'},new_sheet,'
U1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'U2');
T_evap_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_max'},new_sheet,'
V1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'V2');
T_evap_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_evap_mean'},new_sheet,
'W1');
    xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'W2');

p_cond_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_min'},new_sheet,'
X1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'X2');
p_cond_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_max'},new_sheet,'
Y1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'Y2');
p_cond_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'p_cond_mean'},new_sheet,
'Z1');

xlswrite('Matlab_Simulation_Results.xlsx',{'bar'},new_sheet,'Z2');

T_cond_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_min'},new_sheet,'
AA1');
```

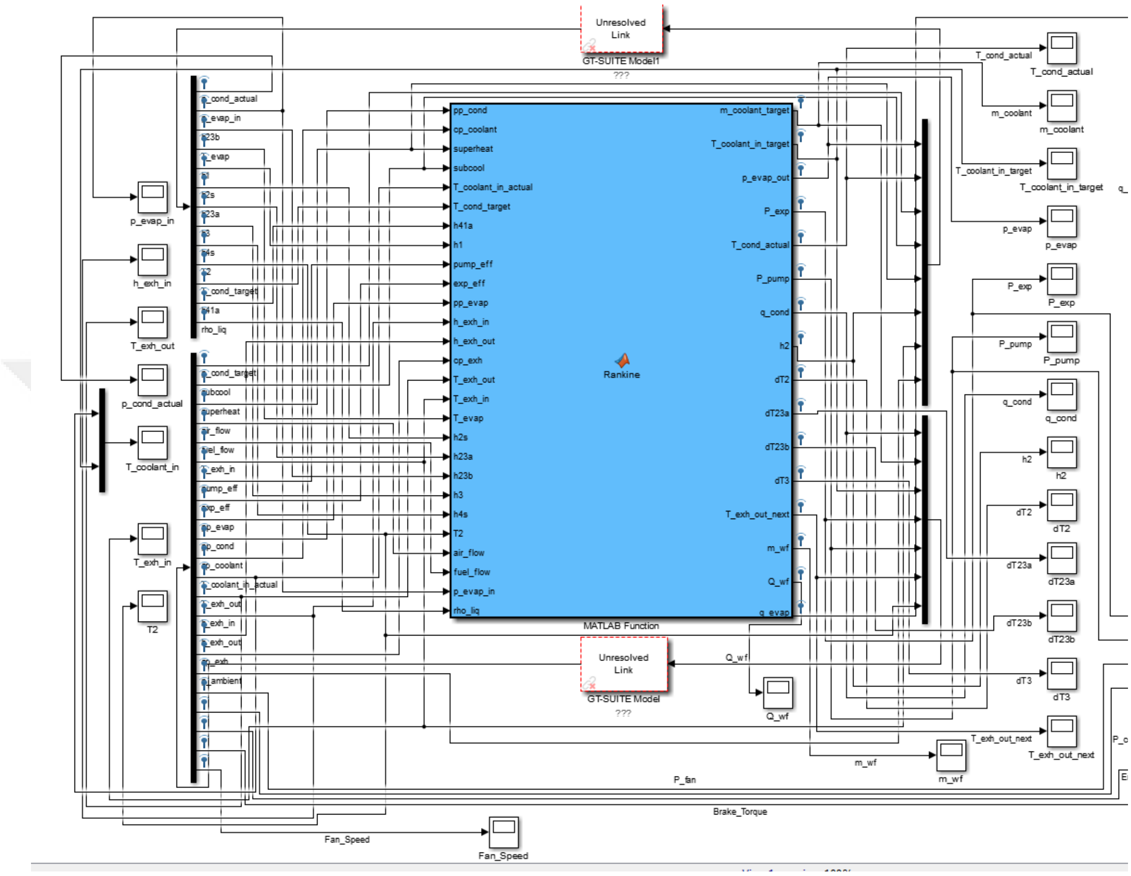
```
xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AA2');
T_cond_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_max'},new_sheet,'
AB1');

xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AB2');
T_cond_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'T_cond_mean'},new_sheet,
'AC1');

xlswrite('Matlab_Simulation_Results.xlsx',{'C'},new_sheet,'AC2');

m_wf_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_min'},new_sheet,'AD
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AD2');
m_wf_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_max'},new_sheet,'AE
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AE2');
m_wf_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'m_wf_mean'},new_sheet,'A
F1');

xlswrite('Matlab_Simulation_Results.xlsx',{'kg/s'},new_sheet,'AF2');

Q_wf_min = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_min'},new_sheet,'AG
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AG2');
Q_wf_max = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_max'},new_sheet,'AH
1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AH2');
Q_wf_mean = ones(1,wf_size(2));

xlswrite('Matlab_Simulation_Results.xlsx',{'Q_wf_mean'},new_sheet,'A
I1');

xlswrite('Matlab_Simulation_Results.xlsx',{'L/h'},new_sheet,'AI2');

for i = 1:wf_size(2)
    s2 = num2str(wf(i));
    disp(strcat('Fluid #',num2str(i),': ',s2,' - ',wf_name{i}));
    Working_Fluid = wf_name{i};

    %% Run Simuink model
```

```
    simOut =
sim('COSMOlogic_Coupling_R2012b_v5_GT','SimulationMode','normal','AbsTol','1e-5',...
                'SaveState','on','StateSaveName','xout',...

'SaveOutput','on','OutputSaveName','yout','SaveFormat',
'StructureWithTime',...
                'SignalLogging','on','SignalLoggingName','logsout');

    logsout = simOut.get('logsout');

xlswrite('Matlab_Simulation_Results.xlsx',wf(i),new_sheet,strcat('A',num2str(i+2)));

xlswrite('Matlab_Simulation_Results.xlsx',wf_name(i),new_sheet,strcat('B',num2str(i+2)));

    P_net = logsout.get('P_net');
    P_net_mean(i) = mean(P_net.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_net_mean(i),new_sheet,strcat('C',num2str(i+2)));

    Brake_Power = logsout.get('Brake_Power');
    Brake_Power_mean(i) = mean(Brake_Power.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Brake_Power_mean(i),new_sheet,strcat('D',num2str(i+2)));

    FE_Benefit(i) = (P_net_mean(i)/Brake_Power_mean(i))*100;

xlswrite('Matlab_Simulation_Results.xlsx',FE_Benefit(i),new_sheet,strcat('E',num2str(i+2)));

    P_exp = logsout.get('P_exp');
    P_exp_min(i) = min(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_min(i),new_sheet,strcat('F',num2str(i+2)));
    P_exp_max(i) = max(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_max(i),new_sheet,strcat('G',num2str(i+2)));
    P_exp_mean(i) = mean(P_exp.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_exp_mean(i),new_sheet,strcat('H',num2str(i+2)));

    P_pump = logsout.get('P_pump');
    P_pump_min(i) = min(P_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_pump_min(i),new_sheet,strcat('I',num2str(i+2)));
    P_pump_max(i) = max(P_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_pump_max(i),new_sheet,strcat('J',num2str(i+2)));
    P_pump_mean(i) = mean(P_pump.Values);
```

```
xlswrite('Matlab_Simulation_Results.xlsx',P_pump_mean(i),new_sheet,s
trcat('K',num2str(i+2)));

    P_fan = logsout.get('P_fan');
    P_fan_min(i) = min(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_min(i),new_sheet,str
cat('L',num2str(i+2)));
    P_fan_max(i) = max(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_max(i),new_sheet,str
cat('M',num2str(i+2)));
    P_fan_mean(i) = mean(P_fan.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_fan_mean(i),new_sheet,st
rcat('N',num2str(i+2)));

    P_coolant_pump = logsout.get('P_coolant_pump');
    P_coolant_pump_min(i) = min(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_min(i),new_
sheet,strcat('O',num2str(i+2)));
    P_coolant_pump_max(i) = max(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_max(i),new_
sheet,strcat('P',num2str(i+2)));
    P_coolant_pump_mean(i) = mean(P_coolant_pump.Values);

xlswrite('Matlab_Simulation_Results.xlsx',P_coolant_pump_mean(i),new
_sheet,strcat('Q',num2str(i+2)));

    p_evap = logsout.get('p_evap_in');
    p_evap_min(i) = min(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_min(i),new_sheet,st
rcat('R',num2str(i+2)));
    p_evap_max(i) = max(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_max(i),new_sheet,st
rcat('S',num2str(i+2)));
    p_evap_mean(i) = mean(p_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_evap_mean(i),new_sheet,s
trcat('T',num2str(i+2)));

    T_evap = logsout.get('T_evap');
    T_evap_min(i) = min(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_min(i),new_sheet,st
rcat('U',num2str(i+2)));
    T_evap_max(i) = max(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_max(i),new_sheet,st
rcat('V',num2str(i+2)));
    T_evap_mean(i) = mean(T_evap.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_evap_mean(i),new_sheet,s
trcat('W',num2str(i+2)));
```

```
    p_cond = logsout.get('p_cond_actual');
    p_cond_min(i) = min(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_min(i),new_sheet,st
rcat('X',num2str(i+2)));
    p_cond_max(i) = max(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_max(i),new_sheet,st
rcat('Y',num2str(i+2)));
    p_cond_mean(i) = mean(p_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',p_cond_mean(i),new_sheet,s
trcat('Z',num2str(i+2)));

    T_cond = logsout.get('T_cond_actual');
    T_cond_min(i) = min(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_min(i),new_sheet,st
rcat('AA',num2str(i+2)));
    T_cond_max(i) = max(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_max(i),new_sheet,st
rcat('AB',num2str(i+2)));
    T_cond_mean(i) = mean(T_cond.Values);

xlswrite('Matlab_Simulation_Results.xlsx',T_cond_mean(i),new_sheet,s
trcat('AC',num2str(i+2)));

    m_wf = logsout.get('m_wf');
    m_wf_min(i) = min(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_min(i),new_sheet,strc
at('AD',num2str(i+2)));
    m_wf_max(i) = max(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_max(i),new_sheet,strc
at('AE',num2str(i+2)));
    m_wf_mean(i) = mean(m_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',m_wf_mean(i),new_sheet,str
cat('AF',num2str(i+2)));

    Q_wf = logsout.get('Q_wf');
    Q_wf_min(i) = min(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_min(i),new_sheet,strc
at('AG',num2str(i+2)));
    Q_wf_max(i) = max(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_max(i),new_sheet,strc
at('AH',num2str(i+2)));
    Q_wf_mean(i) = mean(Q_wf.Values);

xlswrite('Matlab_Simulation_Results.xlsx',Q_wf_mean(i),new_sheet,str
cat('AI',num2str(i+2)));

end
```

APPENDIX D: Snapshot of Simulink Model



CURRICULUM VITAE

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- **B.Sc.** : 2011, Middle East Technical University, Faculty of Engineering, Department of Mechanical Engineering
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