

PERFORMANCE ANALYSIS AND OPTIMIZATION OF R245fa-CYCLOPENTANE ZEOTROPIC MIXTURES IN PARTIAL EVAPORATING ORGANIC RANKINE CYCLES (PEORC) FOR LOW TEMPERATURE HEAT RECOVERY

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ABSTRACT

For low temperature ORC applications, maximum heat recovery and power output are critical. Hydrocarbons used in medium to high temperature applications present excellent heat absorbing characteristics but are limited by their flammability. Combining partial evaporation with a zeotropic blend of alkane-refrigerant as working fluid that combines high temperature glide and high latent heat could enhance system performance. In this study, a partial evaporating ORC (PEORC) using a zeotropic mixture of R245a/Cyclopentane is presented. Influence of vapour fraction and mass fraction on system performance is analysed and optimized performances for a range of heat source temperatures are obtained. PEORC with mixtures achieves the highest heat source utilization at lower vapour fractions. Thermal efficiency and net power output of PEORC using mixtures is higher than that of constituent pure fluids. PEORC with mixtures also minimize the exergy destruction in evaporator and achieves the highest internal and external second law efficiencies. For heat source temperatures ranging from 363K-423K, the performance of PEORC is optimized using Genetic Algorithm and is compared with a standard ORC (SORC). Under optimum operations, PEORC with mixtures outputs 36-65% more power output than SORC with pure R245fa. As heat source temperature increases, PEORC with mixtures and pure R245fa show a decrease in relative improvement of power output over SORC with R245fa. Furthermore, PEORC with mixtures present only 3-5% higher power output than PEORC with pure R245fa. From a thermo-economic standpoint, PEORC using R245fa presents excellent system performance.

1. INTRODUCTION

ORC systems that operate on single, low temperature heat sources are typically of smaller size and capacity. Many of the commercial ORC systems currently in operation are subcritical and operate with pure fluids (Zhai *et al.*, 2015). These systems have lower efficiencies and poor heat extraction potential. Furthermore, adoption of these systems for small scale applications remained a challenge owing to non-availability of efficient small scale turbines.

Recently, development of highly efficient two phase volumetric expanders such as vane expander, screw expander, scroll expander and piston expander have renewed the attention on small scale ORC systems. Out of these, scroll expanders are commercially available and are used in many ORC systems owing to simple structure, two –phase operation and high isentropic efficiencies (Imran *et al.*, 2015). Chang *et al.* (2015) [3] analyzed the experimental performance of a scroll expander using R245fa as working fluid and reported a maximum isentropic efficiency of 73%. Development of such expanders has led to more focus towards cycle architectures deploying two phase expansion. Trilateral cycles (TLC), which use two phase expansion, have been suggested as the best architecture for low temperature heat recovery. However, in TLCs, the latent heat of working fluid isn't utilized leading to lower average heat absorption temperature and higher heat transfer area requirements. Partial evaporating ORCs (PEORC) in which the fluid is heated to a certain vapor quality is emerging

as compromise between the TLC and the fully evaporating standard ORC (SORC) (Lecompte *et al.*, 2013). Compared with a transcritical ORC (TCORC), Lecompte *et al.* (2015) reported 25.6% improved second law efficiency for PEORC. Prior to this, adoption of zeotropic mixtures have been reported to improve power output of SORCs (Andreasen *et al.*, 2014)[6]. Shu *et al.*(2014) suggested mixtures based on hydrocarbons blended with flame retardants to recover engine waste heat ORC. Results showed that zeotropic mixtures do have higher thermal efficiency and lower exergy losses than pure fluids, at a certain mixture ratio. Combining zeotropic mixture with PEORC, Zhou *et al.*(2016) reported 24.7% more output for PEORC with zeotrope over SORC. Very few studies consider the thermo-economic performance and optimization of high latent heat alkanes blended with refrigerants in partial evaporating mode for low temperature heat recovery applications.

In this study, a partial evaporating ORC (PEORC) using a zeotropic mixture of a refrigerant and an alkane is investigated. Two common ORC working fluids R245fa and cyclopentane are selected as working fluids. R245fa/Cyclopentane mixture is able to combine high latent heat variation with high temperature glide. Therefore, this working fluid pair is selected so as to include a wide range of mixture compositions having significantly different latent heat and temperature glide. Influence of vapour fraction and mass fraction on system performance is analysed for PEORC, SORC and TLC. A constrained optimization using Genetic Algorithm is carried out for various heat sources (363K-423K) in the low temperature range. The cycle performance of PEORC with mixtures is compared against with SORC and TLC.

2. SYSTEM DESCRIPTION

2.1 Cycle architecture and working principle

Figure 1 shows the T-s diagram of PEORC using mixtures and pure fluid as working fluids. The system layout is same as that of a simple ORC and consists of an evaporator, pump, condenser and expander. The saturated working fluid from the condenser is pressurised by the pump (5-1). In the evaporator, the working fluid absorbs heat from the heat source and is partially evaporated (1-2-3). The partially evaporate working fluid is then expanded in a two phase expander such as a screw or scroll expander (3-4). The expanded two phase working fluid is then condensed to saturated liquid in the condenser (4-5). When mixtures are used as working fluids, a temperature glide is present in the evaporator and condenser as opposed to the constant temperature heat absorption and rejection in the case of pure fluids.

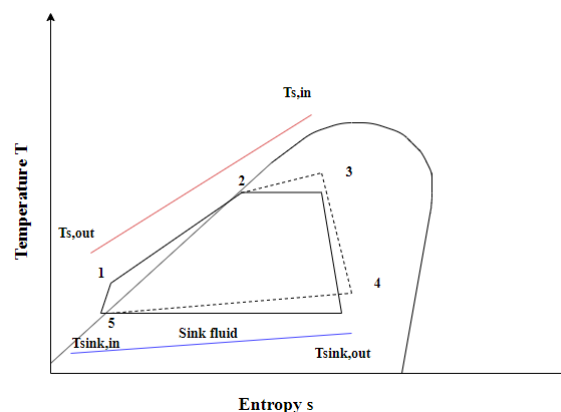


Figure 1: T-s diagram of PEORC with mixtures (dotted lines) and pure fluid (thick lines) as working fluids

2.1 Working fluid characteristics

Cyclopentane and R245fa are selected as the working fluids for this study. The main properties of working fluids are listed in Table 1. R245fa is a common refrigerant used for low temperature ORC applications, whereas cyclopentane is typically used in the medium to high temperature range. As seen from Figure 2, a mixture of cyclopentane and R245fa being an alkane refrigerant zeotropic mixture, possess the advantage of a high temperature glide and latent heat variation. The latent heat of

cyclopentane is almost double that of R245fa. The mixtures also possess high temperature glides for both evaporator and condenser. Therefore, evaluation a mixture of R245fa/cyclopentane for various mass fractions serves as a perfect example for a zeotropic mixture with improved thermal matching and heat absorption characteristics which are desirable for PEORC applications.

Table 1: Thermodynamic properties of working fluids

Working fluid	Molecular mass (g/mol)	Normal boiling point(K)	Critical temperature T_c (K)	Critical pressure P_c (MPa)	GWP	ODP
R245fa	134.05	288.29	427.16	3.651	1030	0
Cyclopentane	70.133	322.40	511.69	4.515	11	0

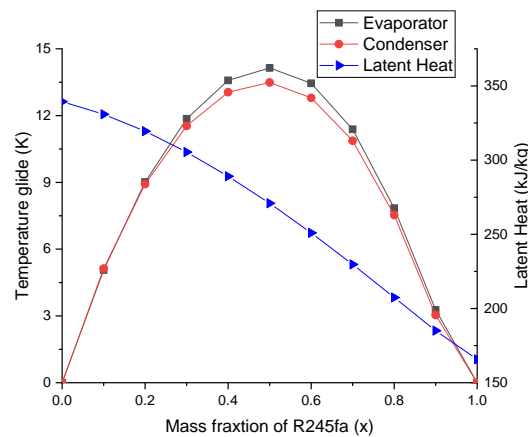


Figure 2: Temperature glide and latent heat variation in R245fa/Cyclopentane mixture.

3. MODELLING METHODOLOGY

The heat source, sink and cycle parameters used in the present study are shown in Table 2. The main thermodynamic model equations are shown in Table 3.

Table 2: Cycle parameters

Parameter		Value
Heat source (water) inlet temperatures	$T_{s,in}$ (K)	363-423
Heat source mass flow rate	m_s (kg/s)	1
ΔT pinch evaporator	ΔT_{evap} (K)	5
ΔT pinch condenser	ΔT_{cond} (K)	5
Isentropic expander efficiency	η_e (%)	70 (Lecompte <i>et al.</i> , 2013)
Isentropic pump efficiency	η_p (%)	80 (Shu <i>et al.</i> , 2014)
Inlet temperature cooling water	$T_{sink, in}$ (K)	298
Outlet temperature cooling water	$T_{sink, out}$ (K)	303
Ambient temperature	T_0 (K)	298
Ambient pressure	P_0 (MPa)	0.1

Table 3: Modelling equations

Parameter	Equations
Net power output (kW)	$W_{net} = W_{exp} - W_{pump}$
Thermal efficiency (%)	$\eta_{th} = W_{net} / Q_{evap}$
Total heat absorbed (kW)	$Q_{evap} = C_{ps} \cdot m_s \cdot (T_{s,in} - T_{s,out})$
Total heat available (kW)	$Q_{total} = C_{ps} \cdot m_s \cdot (T_{s,in} - T_0)$

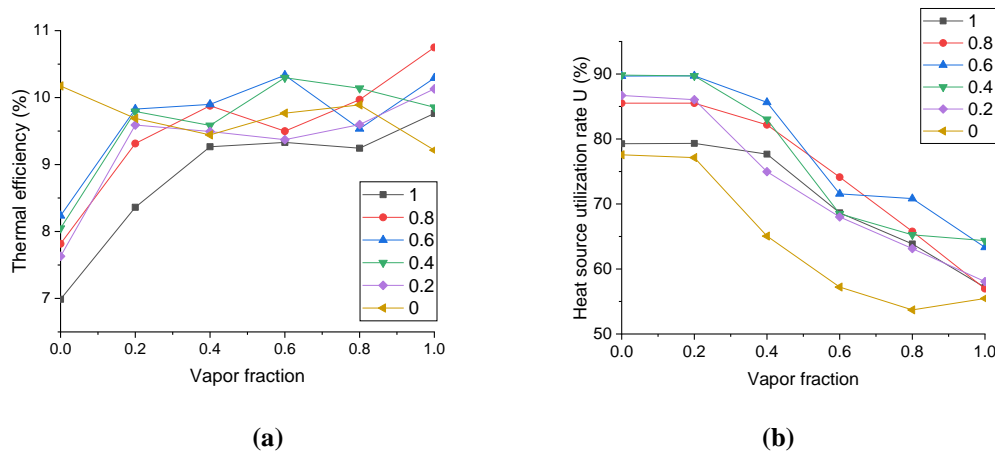
Utilization rate of heat source (%)	$U = Q_{\text{evap}} / Q_{\text{total}}$
Inlet exergy rate of heat source (kW)	$Ex_{S,\text{in}} = m_S e_S = m_S \cdot (h_{S,\text{in}} - h_0 - T_0 (s_{S,\text{in}} - s_0))$
Outlet exergy rate of heat source (kW)	$Ex_{S,\text{out}} = m_S e_S = m_S \cdot (h_{S,\text{out}} - h_0 - T_0 (s_{S,\text{out}} - s_0))$
Internal second law efficiency $\eta_{\text{ex,in}}$ (%)	$\eta_{\text{ex,in}} = W_{\text{net}} / (Ex_{S,\text{in}} - Ex_{S,\text{out}})$
External second law efficiency $\eta_{\text{ex,ext}}$ (%)	$\eta_{\text{ex,ext}} = (Ex_{S,\text{in}} - Ex_{S,\text{out}}) / (Ex_{S,\text{in}} - Ex_{S,0})$
Thermal conductance KA (kW/K)	$KA = Q / \Delta T_{\text{lm}}$
Volume coefficient VC (m ³ /MJ)	$VC = V_{\text{exp,out}} / (h_{\text{exp,in}} - h_{\text{exp,out}})$

Based on the above assumptions and equations, a steady state model is developed in MATLAB using thermodynamic properties of fluids from REFPROP[®] 9.1 software. Energy balance and mass balance is then applied across each components (as a control volume) to determine the system characteristics. The vapour quality q can be between 0 and 1, with 0 being TLC and 1 being SORC. Also the mass fraction of R245fa can vary between 0 and 1, with 0 being pure cyclopentane and 1 being pure R245fa. For the PEORC with mixture, both vapour fraction and mass fraction would assume values between 0 and 1.

4. RESULTS

4.1 Energy analysis

The influence of vapour fraction and mixture composition on the performance of PEORC is analysed for a heat source temperature of 423K. The condensing dew point temperature is fixed at 318K and the evaporating bubble point temperature T_2 is optimized in each case for maximum power output using a Golden section search technique. For mixtures and pure R245fa, the maximum evaporating bubble point temperature is restricted to $0.9T_c$ of R245fa. For pure cyclopentane, this constraint is set to $0.90T_c$ of cyclopentane. As evident from figure 3, the thermal efficiency of PEORC using mixtures exceeds that of SORC and TLC for certain mass fractions. Also, the thermal efficiency of mixtures is higher than that of pure fluids for certain mass fractions of R245fa. This is due to the improved thermal matching in the evaporator. At lower vapour fractions, mixtures achieve the highest heat source utilization, more than pure fluids in PEORC. This improvement in heat extraction is because of the favourable temperature profile developed due to temperature glide in the evaporator. Mixtures in PEORC mode also achieve the highest power output. This is a direct result of the improved thermal efficiency and high heat source utilization for mixtures in PEORC.



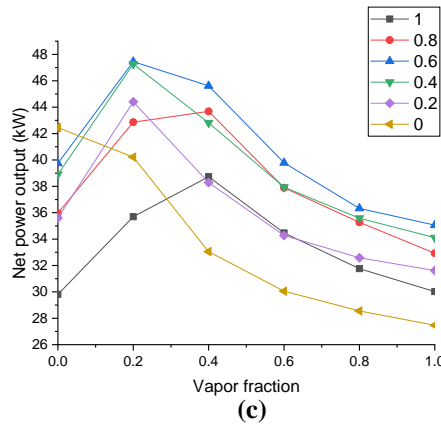


Figure 3: Effect of vapour quality and mass fraction of R245fa on (a) Thermal efficiency (b) Heat source utilization rate and (c) Net power output

4.2 Exergy analysis

Figure 4 presents the effect of vapour fraction and mixture composition on internal and external second law efficiencies. At lower vapour fractions, mixtures exhibit high internal second law efficiencies than that of pure fluids. For mixtures, the lower vapour fractions combined with temperature glide further improves the thermal match. This is the reason for the high internal second law efficiencies in mixtures. High external second law efficiencies are obtained for mixtures and pure fluids owing to the shift in temperature pinch point in the evaporator, which allows for increased heat extraction. As shown in Figure 5, for a given mixture composition there is a vapour fraction that minimises the evaporator irreversibility, thereby leading to high internal second law efficiencies. Therefore, in PEORC using mixtures both mass fraction and vapour quality can be optimized to maximize overall second law efficiency.

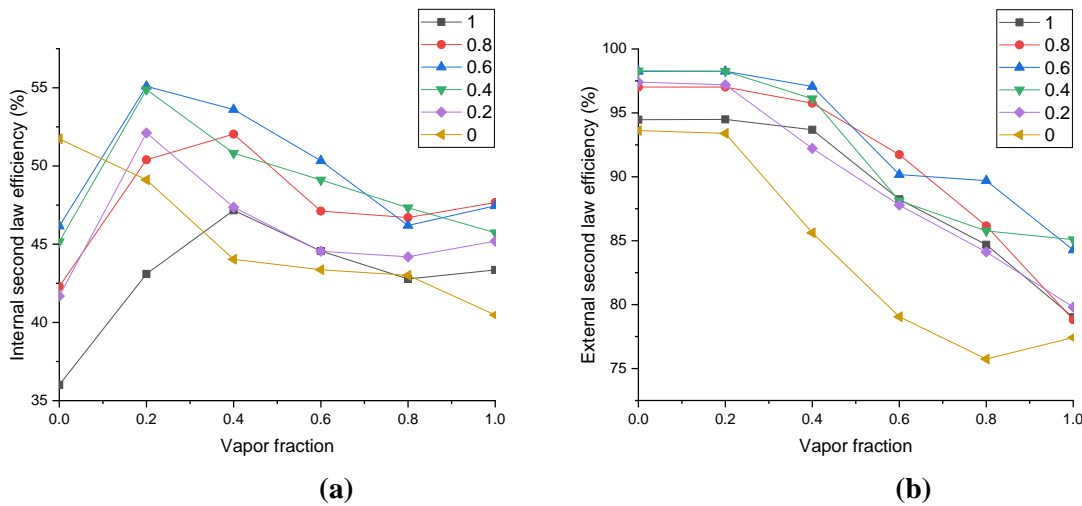


Figure 4: Variation in internal and external second law efficiencies with vapour fraction for various mass fractions of R245fa

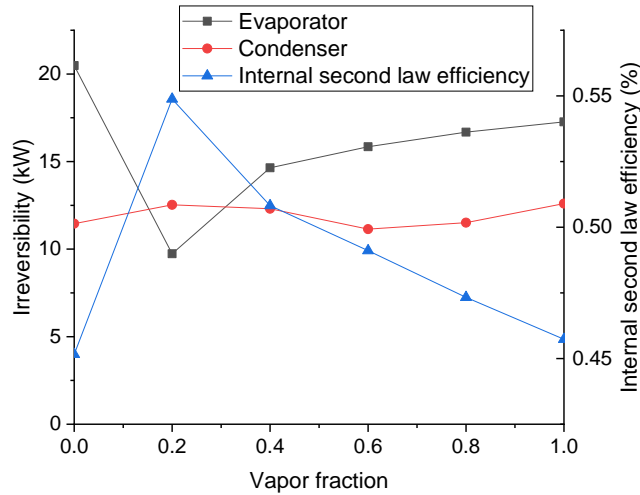


Figure 5: Variation in evaporator and condenser irreversibility and internal second law efficiency with vapour fraction for R245fa mass fraction of 0.4

4.3 Heat exchanger and expander size requirements

Figure 6.a presents the effect of vapour fraction and mass fraction on total heat exchanger KA requirements. Mixtures in PEORC mode show the highest KA requirements. This is due to the increased heat absorption coupled with the decreased logarithmic mean temperature difference in evaporator. SORC shows the minimum overall KA requirement for all the cases. From figure 6.b, mixtures also contribute to higher expander coefficients than pure R245fa. This is due to the higher specific volumes when using mixtures containing cyclopentane. Therefore, the two phase expanders used in mixtures based PEORCs are associated with higher sizes and costs than the turbine expanders used in SORCs.

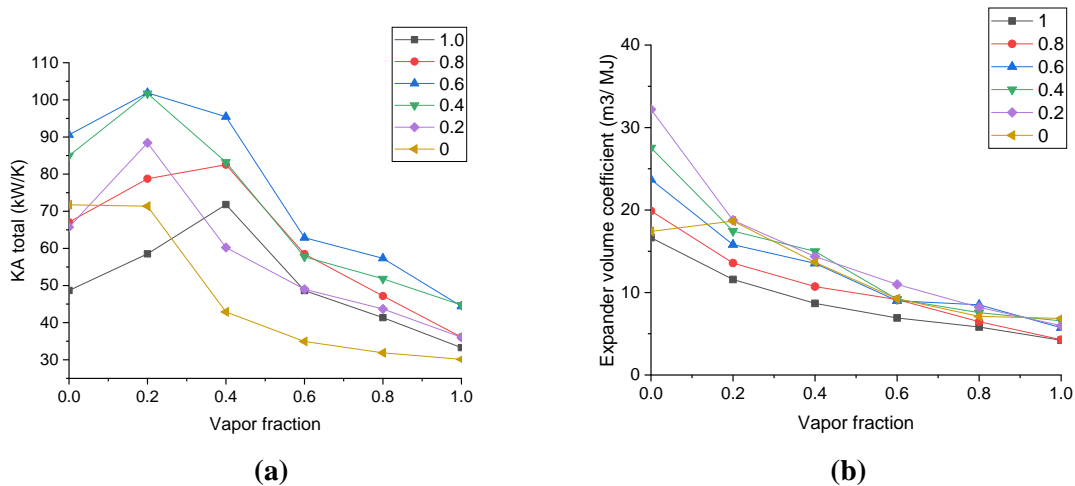


Figure 6: Effect of vapour quality and mass fraction of R245fa on (a) Heat exchanger KA requirements (b) Expander volume coefficient

4.4 Optimization and comparison

For the PEORC with mixtures, the optimization parameters are the evaporating bubble point temperature T_2 , the vapor quality q , mass fraction of R245fa x and condensing dew point temperature T_6 . The range of optimizing parameters along with the cycle design constraints are shown in Table 4. For mixtures and pure R245fa, the maximum evaporating bubble point temperature is restricted to $0.9 T_c$ of R245fa (Zhou *et al.*, 2016). For pure cyclopentane, this constraint is set to $0.9 T_c$ of cyclopentane. The condenser pressure is kept above atmospheric pressure to prevent air leakage into the system. The cycle parameters are optimized using Genetic Algorithm (GA). Net power output is selected as the objective function. The optimized cycle performance is then compared with optimized

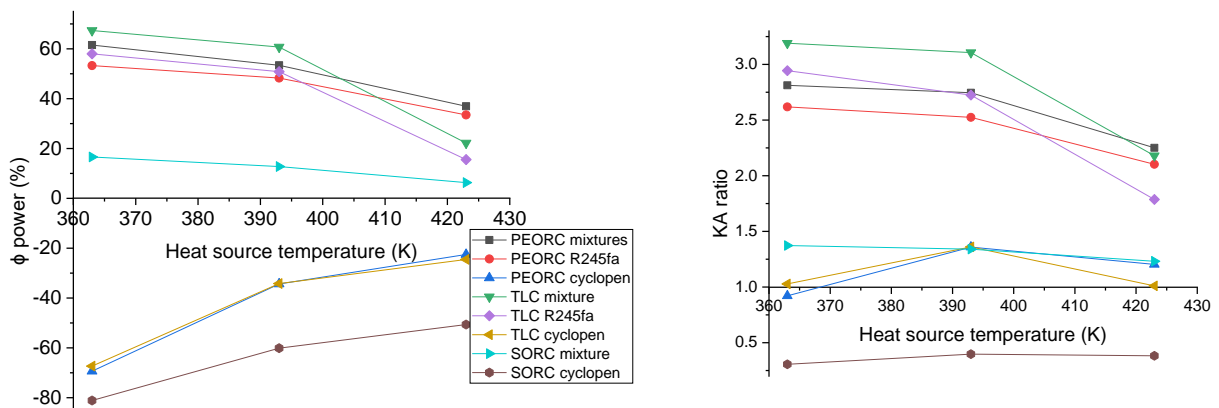
performance of SORC and TLC operating with pure R245fa. Since previous studies (Lecompte *et al.*, 2015) have established that benefits of partial evaporation are the highest for very low temperature heat sources, the simulations are carried out for three typical low heat source temperatures of 363K, 393K and 423K.

Table 4: Optimizing parameters and constraints

Cycle Parameters/ constraints	Range/Value
Evaporating bubble point temperature T_2	323-393K
Condenser dew point temperature T_{cond}	308K – 333K
Mass fraction of R245fa x	0.01-0.99
Vapor quality q	0.01-0.99
P_{cond}	≥ 1.50 bar
GA parameters	
Population size	40
Maximum generations	400
Function tolerance	0.001

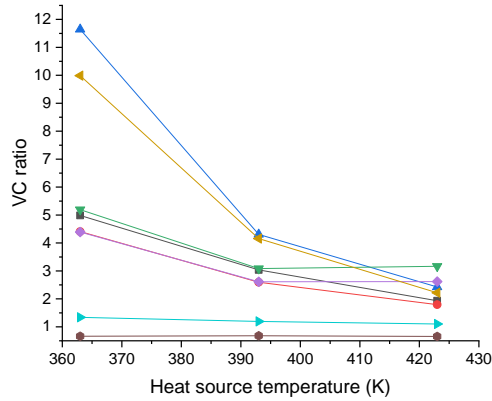
Figure 7 shows the optimized results of PEORC, TLCand SORC with pure R245fa- SCORC as the baseline for comparison. PEORC with mixtures outputs 36-65% for more power compared to SORC with pure R245fa for the heat source temperatures investigated. At lower heat source temperatures of 363K and 393K, TLC with mixtures performs the best, followed by PEORC with mixtures and pure R245fa. However, TLC presents poor heat exchanger and expander economy owing to the higher KA ratios and VC ratios over R245fa based SORC. Also, PEORC with mixtures present only 3-5% higher power output than PEORC with pure R245fa. This could be because of the higher condensing temperatures in mixtures than pure R245fa for condenser pressures above atmospheric pressure. Cyclopentane based TLC, SORC and PEORC show poor thermodynamic performance owing to higher condensation temperatures.

PEORC with pure R245fa exhibits intermediate KA values, 7-8% and 4-18% lower than PEORC and TLC using mixtures. In comparison with pure fluids, heat transfer performance of mixtures is worse than that of pure fluids. This is due to the limitation in phase change process due to diffusion and degradation of transport properties (Radermacher,2005). Analysing the effect of transport properties such as thermal conductivity, diffusivity and viscosity on heat exchanger area requires a detailed heat exchanger design analysis, which is beyond the scope of this paper. It can be inferred that the higher KA requirements in mixtures would lead to higher heat exchanger area requirements. Also, the VC values associated with pure R245fa in PEORC are also lower (7-12% and 15-43% lower than that of PEORC using mixtures and TLC using mixtures). Therefore, when operating under restrictive conditions PEORC with pure R245fa devlivers excellent system performance.



(a)

(b)



(c)

Figure 7: Optimized results of PEORC, SORC and TLC for various heat source temperatures (same legend for all plots).

5. CONCLUSION

A PEORC system using zeotropic mixture that combines partial evaporation with temperature matching is presented. R245fa/cyclopentane mixture that combines the advantage of high variation in latent heat and temperature glide is selected as the working fluid. Influence of vapour fraction and mass fraction on system performance is analysed and optimized performances for a range of operating conditions are obtained. The cycle performance is compared with SORC using pure R245fa as baseline.

1. At lower vapour fractions, PEORC with mixtures achieve the highest net power output and heat source utilization rates.
2. At optimum mass fractions, PEORC with mixtures minimize the exergy destruction in evaporator and achieves the highest internal and external second law efficiencies.
3. Heat exchanger requirements and expander economy of PEORC using mixtures is quite poor when compared with SORC.
4. Under optimized conditions, PEORC with mixtures deliver 36-65% for more power output when compared with SORC with pure R245fa for the heat source temperatures investigated. As heat source temperature increases, PEORC with mixtures show a decrease in relative performance over SORC with R245fa. Furthermore, PEORC with mixtures present only 3-5% higher power output than PEORC with pure R245fa. PEORC with pure R245fa also exhibits intermediate KA values, 7-8% and 4-18% lower than PEORC and TLC using mixtures. Overall, PEORC with R245fa shows promising system performance than that of mixtures

NOMENCLATURE

C_p	specific heat at constant pressure	(kJ/kg K)
e	specific exergy	(kJ/kg)
Ex	exergy	(kJ)
h	specific enthalpy	(kJ/kg)
KA	thermal conductance	(kW/K)
m	mass flow rate	(kg/s)
P	pressure	(MPa)
Q	heat transfer rate	(kW)
q	vapor fraction	
s	specific entropy	(kJ/kg K)
T	temperature	(K)
U	utilization rate of heat source	(%)
VC	expander volume coefficient	(m ³ /MJ)
W	power	(kW)
x	mass fraction of R245fa	

Subscript

c	critical point
cond	condenser
evap	evaporator
exp	expander
in	inlet
lm	log mean temperature
max	maximum
out	outlet
s	source
wf	working fluid

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