THE IMPACT OF WORKING FLUID CHARGE ON PERFORMANCE OF ORGANIC RANKINE CYCLE USING ZEOTROPIC MIXTURE UNDER DESIGN CONDITION

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ABSTRACT

Mass-based analysis of thermodynamic cycle can be a link to realize the matching between the working fluid properties, performance of components, and operation parameters. The present paper proposes a working fluid charge-oriented analysis for ORC systems operated with zeotropic fluid mixture. It combines the fundamental equations with the working fluid mixture variation analysis during heat transfer processes, focusing on evaporator and condenser as the phase-change components. This proves to be an effective way to investigate the impact of working fluid mass on performance of ORC systems. Results indicated that liquid-phase zones in both heat exchangers account for more than 60% of total working fluid mass. Since the largest composition shift occurs during condensation, this relation affects the masses and composition shifts in other components as well as the overall system. Moreover, the relationship between the total mass and composition shift of zeotropic mixture are analyzed. It is found that the increase of total mass of working fluid leads to a decrease of mass in the two-phase regions and an increase of mass in the single-phase zones. It therefore causes a reduction of the average composition shift in the system. The system performance analysis shows the highest net output work of 2.42 kW, which occurs when the total mass of working fluid rises to 130% of the design value. However, further increases in mass will have a negative impact on system performance.

1 INTRODUCTION

The Organic Rankine Cycle (ORC) is an effective way to enable power generation from low-grade heat sources. Previous ORC-related research paid a lot of attention to system modelling and its performance analysis under various conditions. It can be investigated by means of model-based simulations with commercial and in-house codes. Indeed, the operating of an organic Rankine cycle system under different conditions is a mass distribution process of a certain amount of the working fluid between different main components in the closed cycle. The heat source/sink, and the load demand of the system are the external conditions of such mass distribution processes. Therefore, the distribution of working fluid mass is the link for study of the ORC system performance to realize the matching between the performance of main components and the system operation parameters. Theoretical model should be developed for investigation the mass distribution in detail, and the influence of different working fluid charge amount on the performance of ORC system should be also investigated in depth through the established model. Such researches has important theoretical significance and application value for the promotion of the ORC technology. An innovative working fluid charge-oriented model, which focus on the total mass of working fluid in the system as an indicator of analysis, was firstly proposed by Rossi (1995) for a refrigeration system. The total mass of refrigerant in the system served as a convergence index for developing the model solution algorithm. Afterwards, a more precise performance prediction model was developed by Shen *et al.* (2006,2009) to estimate the impact of different mass of refrigerant. Due to the similarity of refrigeration systems to ORC technology, the existing methodologies can be considered as ORC-related and adapted to ORC research. Ziviani *et al.* (2016) developed charge-sensitive models for two small-scale ORC systems, which were thoroughly validated by experiments. Results indicated that the proposed model showed satisfactory accuracy in predicting cycle efficiency. Another investigation was carried out by Liu *et al.* (2017) in which an ORC unit with 3 kW rated output power was modelled, and the impact of different working fluid mass on the performance of the system was analyzed in detail. In addition to that, Pan *et al.* (2018) investigated the same ORC unit where the repartitions of the working fluid mass in each component are calculated in detail. Dickes *et al.* (2018) studied the accuracy of the heat exchanger models, where the total working fluid mass in the system was used as an indicator for validation of the established model. Calculations based on several state-of-the-art heat transfer correlations as well as void fraction models were compared with experimental data. Moreover, another article by Dickes *et al.* (2018) introduced a weight based online measurement method to measure the fluid mass in heat exchangers. The inlet- and outlet pipe of the heat exchanger are replaced by a hose, and the heat exchanger is suspended, so as to indirectly measure the real-time mass change of the working fluid according to the weight-change of heat exchangers. Such improvement makes it possible to obtain a more precise prediction of the working fluid mass.

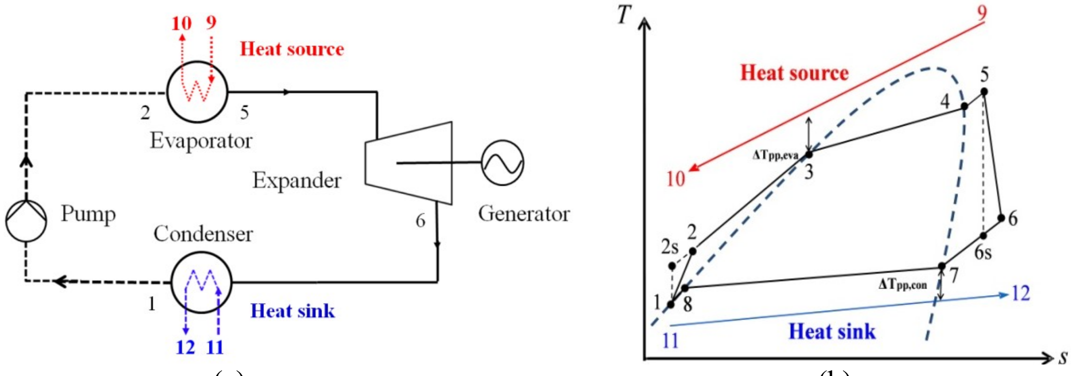
In recent years, the application of zeotropic mixtures has become an important branch ORC research. However, only a few scholars considered the impact of composition shift on the estimation of the optimal total mass and composition of the working fluid. Narasimhan *et al.* (2010) proposed a method for estimating the composition of the mixture to be filled into the ORC in order to get the desired composition during operation. The linear fitting relationships between the local composition and the global composition were obtained based on experimental results. Xu *et al*. (2011) pointed out that the liquid-phase retention caused by the velocity difference between both phases was the main reason for the composition shift. Zhao *et al.* (2014) indicated that the composition shift of the mixture will cause a significant decrease in the output power of the ORC system.

Since previous working fluid charge-oriented performance analysis for ORC systems has only been introduced for systems using pure fluids, the present paper applies modelling of the ORC system. This work focuses on the analysis of the mass of working fluid and the composition of zeotropic mixture and thus takes into account the composition shift. The developed model-based simulation and optimization has been used to investigate a small-scale ORC system using R245fa/R365mfc as working fluid by analyzing the relationship between total mass and average composition shift of the zeotropic mixture. Moreover, the impact of total mass of working fluid on the system performance around the design condition has been investigated, considering the phenomenon of composition shift during the heat transfer process in heat exchangers.

2 MATERIALS AND METHOD

2.1 System description

The schematic diagrams of the ORC system considered in this study and the relevant *T-s* diagram have been illustrated in Figures 1(a) and (b), respectively. As shown in Figure 1, the zeotropic mixture is compressed by the pump (1-2), it absorbs heat from the heat source in the evaporator (2-5). The working fluid vapour, at high temperature, is expanded in the expander (5-6) to generate mechanical energy. The low-pressure vapour exits the expander and enters the condenser to reject heat (6-1) to the heat sink. The liquid-phase working fluid is then again directed to the pump and the cycle is closed. Figure 1 (b) shows the heat input in the evaporator (2-3-4-5) and heat output (6-7-8) in more detail, the phase-changes are simplified by straight lines for readability purposes. Table 1 summarizes the main operating parameters of the system in this study.



(a) (b)

Figure 1: (a) Schematic diagram of the ORC system (b) *T-s* diagram for the ORC system.

Table 1: Design parameters of the ORC system using R245fa/R365mfc as working fluid.

Parameter	Value	Unit	Parameter	Value	Unit
T_9	423	K	ΔT_{sub}	5	K
$\dot{m}_9$	0.33	kg/s	$\Delta T_{pp,eva}$	≥5	K
T_{11}	293	K	$\Delta T_{pp,con}$	≥5	K
ΔT_{sup}	20	K	η_{pp}/η_{exp}	0.75	-

2.2 Thermodynamic models

The numerical model of the ORC system was combined with sub-models for all main components. Considering that the mass of the working fluid in pump and expander can be neglected, a lumped parameter model was used to describe the working fluid for pump and expander. The subsequent calculation did not consider a specific design, type or construction of these two components. On the other hand, the heat transfer process in both heat exchangers was analysed in detail through steady-state models. For the single-phase zones in both heat exchangers, correlations for convection heat transfer process in a horizontal tube modified by resistance coefficient (*Qian*, 2002) can be used for calculate the heat transfer coefficient. Moreover, the correlation for boiling heat transfer to saturated fluids in convective flow proposed by *Chen* (1966) and the correlation for condensation heat transfer process of outside tubes proposed by *Kern* (1958) are used for the estimation of heat transfer coefficient in two-phase zones in evaporator and condenser, respectively. The required heat transfer areas of each zone was determined by the logarithmic mean temperature difference (LMTD) method and pinch point analysis; here, only the sub-critical pressure are considered in this analysis. Based on the physical properties of the heat source and sink, a finned tube heat exchanger was used as evaporator (gaseous heat source), while a shell and tube exchanger was used as a condenser (liquid heat sink). It should be noted that the selection of the combination of a lumped parameter model with the steady-state model is based on a trade-off between the computational efficiency and model accuracy for the estimation of the working fluid charge level in the ORC system. The analysis of the system performance under both design condition were derived from these models. It is worth noting that the solution scheme is based on the optimization of mass flow rate of working fluid to maximize the system output work and passed through the validations of the heat transfer area of both heat exchangers. The input values for the calculation process are the design values listed in Table 1 as well as the initial set value of the evaporation temperature. The detailed calculations and formulae of the thermodynamic processes as well as heat transfer correlations have been described in previous papers (Liu *et al.* 2017 and Pan *et al.* 2018).

All the above mentioned processes are implemented in Matlab 2019, and the relevant physical properties of the working fluid mixture were obtained from Refprop 9.1 developed by NIST (Lemmon *et al.* 2013). It should be pointed out that due to a lack of detailed experimental data for the concerned binary mixture, the calculated properties through Refprop 9.1 are estimates by similar fluids. Moreover, the interaction parameters have not been fitted to their model even though data exist. According to the comments to the latest version Refprop 10.0 (Lemmon *et al.* 2018), the scheme works fairly well, especially for the refrigerants. It breaks down with dissimilar fluids and eventually will produce large interaction parameters. Moreover, the transport equations of the two pure fluids considered in this paper are further modified in the new version Refprop 10.0. The detailed methodology for the calculation of transport properties of mixtures used in the Refprop can be found in the NIST internal report (Chichester *et al.* 2008). However, this does not significantly affect the reference value of the methodology recommended in this paper and the qualitative laws derived from the study.

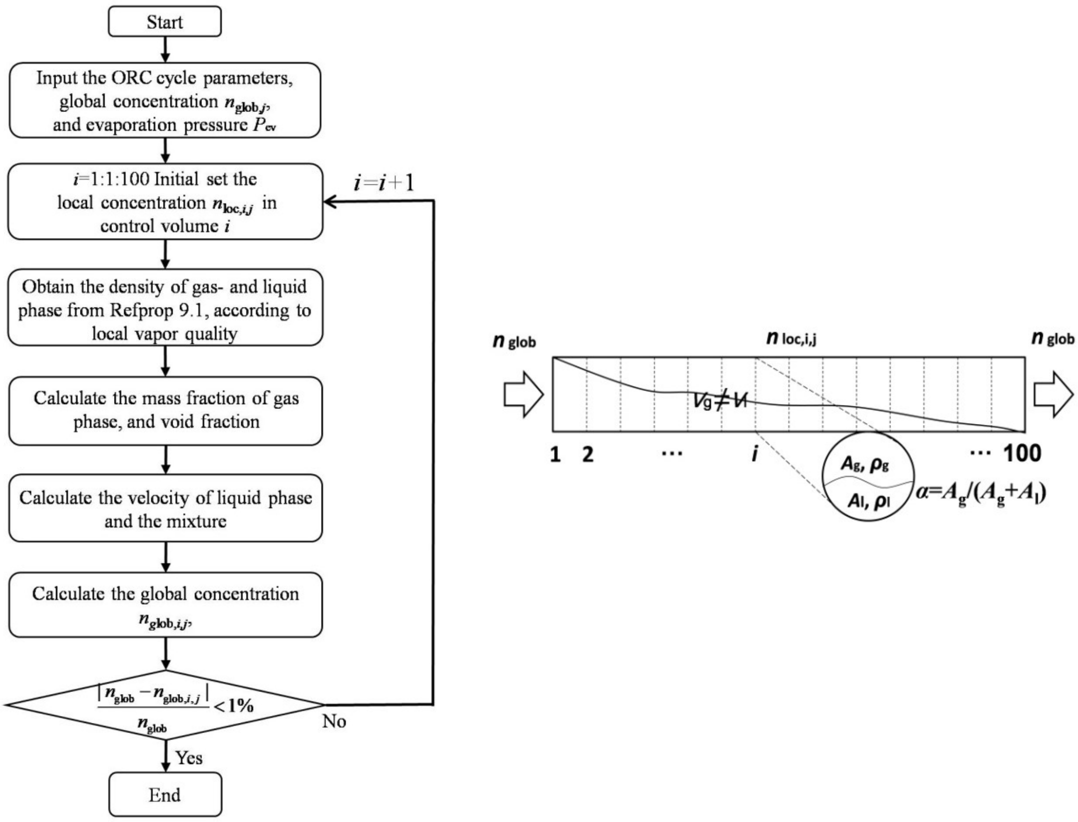
2.3 Estimation the composition of the zeotropic mixture in the two-phase zone

The conservation of the total mass of the working fluid is an important constraint for the design and performance analysis of the thermodynamic cycles with zeotropic mixtures. Therefore, this work further combines the working fluid charge oriented modelling with the composition shift analysis for the zeotropic mixture. Based to previous investigations, the key issue of such a model is the estimation of the mass of the working fluid in the two-phase region of the heat exchangers. It is well known that in the absence of leakage, the mass of the working fluid in each component is conserved at steady-state. However, due to the differences between flow velocity of gas-phase and liquid-phase, the initial global mass composition ($n_{\mathrm{glob},j}$) into the system and the local mass composition ($n_{\mathrm{loc},i,j}$) of the working fluids at each point during the two-phase heat transfer process are different. In this work, different compositions of the zeotropic working fluid mixture have been calculated in dependence of the mass fraction of the fluid with the lower boiling point (R245fa). The local mass composition of the working fluid in the two-phase zone has been calculated using a finite volume method. The two-phase zone of both heat exchangers was divided into several units, according to the vapour quality. To manage the trade-off between the accuracy and efficiency of the model, the calculation interval of vapour quality in this work was set to 0.01 and thus 100 finite volume elements. Figure 2 illustrates the programme flow chart for the calculation of the local mass composition in the two-phase zone. Moreover, as the starting value for the iterative calculation process, an optimal global mass composition of the working fluid was estimated for maximising the net power output of the system.

Since using either the zeotropic mixture or the pure working fluid does not result in a noticeable difference in the thermodynamic optimisation process, estimation of the optimal global mass composition can be made in accordance to our previous work (Liu *et al.* 2017). It was found that the net output work of the system is closely linked with the working fluid composition, a maximum value of 2.268 kW was achieved at 0.605 mass fraction of R245fa. Therefore, the optimal global mass composition under the design conditions is found to be a mass fraction of 0.605/0.395 for R245fa/R365mfc. Table 2 summarises the other related operation parameters of the system at this particular mass fraction and Figure 2 shows the flow chart of the iterative estimation procedure of local mass compositions in two-phase zone. The formulae used in the calculation process, can be found in literature (*Smith*, 1969).

Table 2: Operation parameters of the ORC system using R245fa/R365mfc as working fluid.

Parameter	Value	Unit	Parameter	Value	Unit
T_{10}	358	K	$\dot{m}$	0.073	kg/s
T_{12}	298	K	n_{glob}	0.605	-
$\overline{T}_{\mathrm{eva}}$	387	K	W_{net}	2.268	kW
$\overline{T}_{\mathrm{con}}$	316	K	η_{th}	11.3	%



(a) (b)

Figure 2: (a)Flow chart and (b)diagram for estimation of the local mass composition in two-phase zones.

3 RESULTS AND DISCUSSIONS

The established model has been used to analyse the mass distribution of the working fluid and its influence on the performance of the system under the design condition. First, the total mass of the working fluid at the optimal global mass composition was calculated, and the relationship between mass and composition in each heat transfer zone was analyzed. Afterwards, the influence of the total mass of the working fluid on the composition shift phenomenon was discussed. Finally, the impact of the working fluid mass on performance of the ORC system, which operated under the design condition was analyzed.

3.1 Mass distribution of the working fluid under the design condition

The calculation results of the working fluid mass related parameters under the design condition have been summarized in Table 3. The global mass composition of the working fluid obtained from the preliminary thermodynamic optimization was found to be 0.605, while the calculated real average mass composition in system was 0.589, and the composition shift of working fluid under this condition was 1.83%. Moreover, the calculated heat transfer area of the evaporator was 6.20 m^2, while that of the condenser was 2.04 m^2. The calculated total mass of working fluid in the system was found to be 15.2 kg, including 6.38 kg in evaporator and 8.82 kg in the condenser. It has been found that most of the working fluid accumulates in the preheat zone of the evaporator and the sub-cooling zone of the condenser. In particular, the mass of the working fluid in these two zones accounted for more than 60% of the total mass of the total working fluid amount. Therefore, the heat transfer process in these two zones has a significant impact on the performance of the heat exchanger. Moreover, the evaporation zone in the evaporator and the condensing zone in the condenser contained the second-largest amount of the total mass of working fluid, i.e., 10% and 22%, respectively. The mass of the working fluid distributed in the superheat zone of the evaporator and the de-superheating zone of the condenser was calculated to be relatively small, accounting for only 2% and 4% of the total mass of working fluid, respectively. It is worth noting that although the heat transfer area of the evaporator is larger than that of the condenser, the mass of the working fluid in the evaporator was found to be smaller than that of the condenser. The reason for this phenomenon is further discussed in the following section.

Table 3: Mass and mass composition distribution of working fluid under the design condition (n_{glob}=0.605).

	Zone	Area (m^2)	%	Volume (m^3)	Mass (kg)	%	Average composition	Relative Composition shift %
Evaporator	Preheat	3.71	43	0.004	4.56	30	0.605	0
	Evaporation	2.35	27	0.004	1.67	10	0.578	4.46
	Superheating	0.14	2	0.002	0.15	2	0.605	0
	Σ	6.20	72	0.010	6.38	42	-	-
Condenser	De-superheating	1.26	15	0.010	0.62	4	0.605	0
	Condensation	0.91	11	0.003	3.34	22	0.556	8.10
	Subcooling	0.23	2	0.004	4.86	32	0.605	0
	Σ	2.40	28	0.017	8.82	58	-	-
Total		8.60		-	15.20		0.592	2.09

3.2 The relation between mass and composition of the working fluid

In the heat transfer process of the two-phase zone, the composition shift of the cross-section can be calculated by the difference between the global mass composition and the local mass composition. As shown in Table 3, the composition shift in the condensation zone (8.10%) was greater than that in the evaporation zone (4.46%). Therefore, the proportion of the mass in the condensation zone was the main factor that affected the composition shift in the system. The higher the mass of the working fluid in the condensation zone, the greater the difference between the global mass composition and the local mass composition. Furthermore, an increase in the working fluid mass in both the preheat- and evaporation zone, of the evaporator had only little effect on the results of the composition shift. Moreover, due to the small mass of working fluid in the superheating zone of the evaporator and the de-superheating zone of condenser, their influence on the composition shift can be neglected.

According to the above analysis, the composition shift of the entire system can be reduced by increasing the working fluid mass in the liquid-phase zone of both heat exchangers and by decreasing the proportion of working fluid mass in the condensation zone, in the condenser. This adaption can be realized by adjusting the flow rate of both the working fluid and the cooling water. Figure 3 illustrates the negative correlation of the composition shift of the entire system with the increase of the mass flow rate of the cooling water. The mass of the working fluid accumulated in the condenser was seen to decline from 11.1 kg to 8.7 kg when the mass flow rate of the cooling water rose from 0.7 kg·s^{-1} to 1.5 kg·s^{-1}. The average composition shift in the overall system declined from 2.09% to 1.65% and can be explained by analysing the heat transfer process. With the increase in mass flow rate of cooling water, the heat transfer coefficient in the condensation zone increases significantly. Consequently, the necessary heat transfer area was less, the amount of transferred heat in the condenser remained nearly constant, and the mass of the working fluid in the condensation zone decreased. Since the mass flow rate of the cooling water had no apparent influence on the evaporator side, the mass of the working fluid accumulated in the evaporator did not change significantly. Therefore, the calculated mass of the working fluid in the entire system decreased.

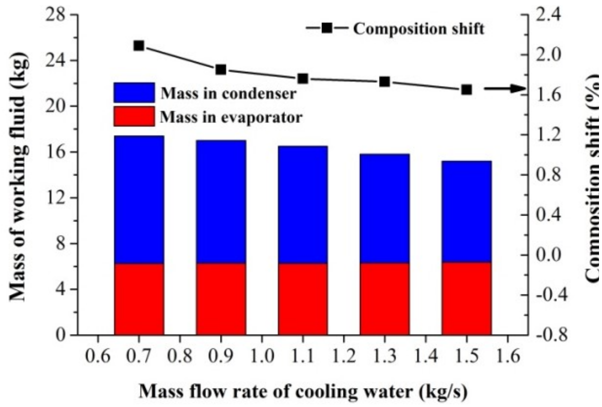


Figure 3: Variation of mass composition shift and working fluid mass.

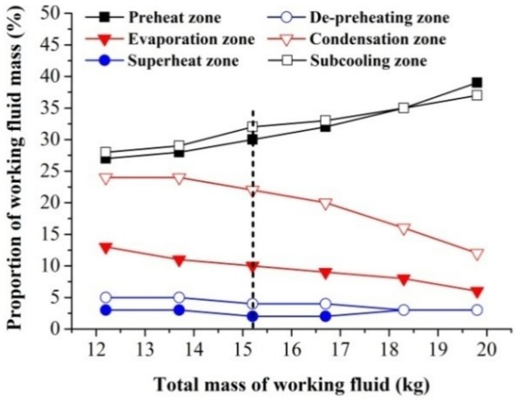


Figure 4: Variation of mass proportion in different zones in heat exchangers.

Furthermore, the variation of the mass ratio of the working fluids in the different zones and independence of the total mass, was studied. The influence of 15.2 kg (reference value) of working fluid mass with intervals of ±10%, was observed. As shown in Figure 4, increasing the amount of working fluid resulted in a gradual decrease of the mass in the two-phase zone of both heat exchangers. In contrast to that, the mass in the single-phase zones, increased significantly, especially in the liquid-phase. The proportion of the mass in the subcooling zone rose from 28% to 42% when the amount of the working fluid increased from 12.2 kg to 19.8 kg. The increase of the working fluid mass in the liquid-phase zones promoted the reduction of the composition shift in the entire system.
Figure 5 illustrates the trend of the global mass composition and the calculated average mass composition. It can be found that an increase in the amount of working fluid had a positive effect on the reduction of the composition shift. More specifically, a 20% increase in the mass of working fluid (18.3 kg) results in a reduction of the difference between global mass composition and average mass composition down to nearly 1%. However, the effect of any further increase in the mass was no longer significant.

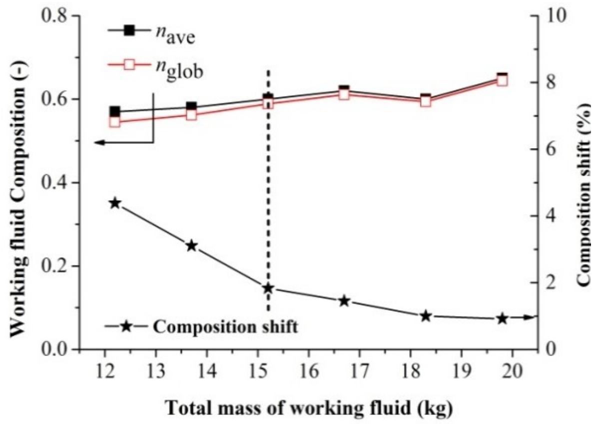


Figure 5: Variation of mass composition shift of the working fluid.

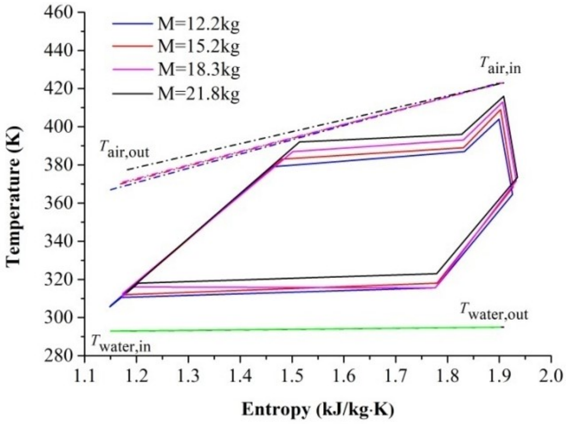


Figure 6: *T-s* diagram of ORC system with different total mass of working fluid.

3.3 The impact of different working fluid mass on the performance of the system

The calculated performance indicators of ORC with different working fluid mass are summarized in Table 4 and the relevant *T-s* diagrams of the four cycles which working nearly the design point with different total mass of working fluid are shown in Figure 6. It is clear that with the increase in total mass of working fluid, the heat transfer area in the two-phase zone in heat exchangers is covered by liquid-phase, causing the mass flow rate of working fluid to rise to ensure adequate heat transfer amount between working fluid and heat source/sink. The average evaporation pressure and the average condensation pressure of the system increase accordingly. As shown in Figure 6, the average evaporation pressure rises from 1.16 MPa to 1.52 MPa when the total mass of the working fluid goes from 12.2 kg to 21.8 kg. However, this increase trend will be limited by the minimum pinch temperature difference of the heat exchanger. It was found that with the increase of the total mass, the mass flow rate of working fluid first goes up from 0.072 kg/s to 0.074 kg/s, then down to 0.069 kg/s. The output work of the expander and the power consumption change with the same trend. Meanwhile, since the enthalpy of the working fluid in the saturated liquid-phase was much less affected by the pressure than the saturated gas-phase, the variation amplitude of power consumption of the pump was less than the output work of the expander. Hence, through this process, the net output work of the system was firstly rises and then beings to decline after reaching the highest value. As shown in Table 4, the highest net output work obtained was 2.42 kW when the total mass of working fluid was 19.8kg, and the relevant thermal efficiency was nearly 12.33%. Therefore, an increasing the total mass of the working fluid within a certain range proved to be an effective way to improve system performance. However, further increases can also have a negative impact on system performance.

Table 4: Performance of the ORC system under different working fluid mass.

M_{wf}(kg)	$\overline{P}_{eva}$(MPa)	$\overline{P}_{con}$(MPa)	$\dot{Q}_{eva}$(kW)	$\dot{W}_{exp}$(kW)	$\dot{W}_{pp}$(kW)	$\dot{W}_{net}$(kW)	η_{th}(%)
12.2	1.16	0.19	19.83	2.22	0.05	2.17	10.90
13.7	1.22	0.2	19.86	2.30	0.06	2.24	11.28
15.2	1.31	0.21	20.07	2.33	0.06	2.27	11.30
16.7	1.38	0.22	20.13	2.41	0.07	2.34	11.62
18.3	1.42	0.22	20.28	2.48	0.07	2.41	11.88
19.8	1.50	0.23	19.63	2.49	0.07	2.42	12.33
21.8	1.52	0.23	19.35	2.02	0.07	1.95	10.31

4 CONCLUSIONS

This paper proposes a working fluid mass-based performance analysis for an ORC system using zeotropic mixture under the design condition. The main conclusions of this study are summarized as follows:

1. An increase of working fluid mass in the single-phase zone and a decrease of working fluid mass in the two-phase zone play an active role in reducing the composition shift of the overall system. For the system in this study, the overall average composition shift was seen to decline from 2.09% to 1.65% as the mass of working fluid in the condenser declined from 11.1 kg to 8.7 kg.
2. There are two benefits of increasing the total mass of working fluid. Firstly, increasing the mass of working fluid was seen to decrease the mass in the two-phase zone of both heat exchangers and noticeably increase the mass in the single-phase zone. Consequently, a reduction of the average mass composition of working fluid was observed.
3. Moreover, proper increasing the mass of working fluid proved to be an effective way to improve system performance. Results indicated that the highest net output work occurred when the mass of the working fluid rose to 130% of the design value. Of course, this should also be combined with the economic analysis of the system for a comprehensive consideration.

Because the estimation of mass of working fluid involves several branches of study, the distribution of working fluid mass and the impact on system performance may vary greatly in different systems. Therefore, extensive research catered to specific systems is needed. It should be pointed out that because the shell and tube heat exchanger has the function of liquid storage, there is no reservoir in the system discussed in this paper. In fact, since there is no obvious heat transfer between the working fluid and other fluid in the reservoir, the existence of the reservoir will only affect the economic and dynamic performance of the system. The detailed discussion will be carried out in our future researches. Moreover, this present preliminary study can be extended and validated by the development of an effective online test method for the working fluid mass to promote experimental research.

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