Using a cubic equation of state to identify optimal working fluids for an ORC operating with two-phase expansion using a twin-screw expander

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ABSTRACT

For waste-heat recovery applications, operating an organic Rankine cycle (ORC) with two-phase expansion has been shown to increase the utilisation of the waste-heat stream, leading to a higher power output compared to a conventional ORC with single-phase expansion. However, unlike the conventional ORC, working-fluid selection for an ORC operating with two-phase expansion has not been explored in detail within the literature. Therefore, the aim of this paper is to explore which working-fluid parameters make a particular working fluid suitable for this type of cycle. This is conducted by coupling a thermodynamic model of the cycle with the Peng-Robinson cubic equation of state. Moreover, the effect of the expander volumetric ratio on the expander isentropic efficiency is accounted for using a performance model for a twin-screw expander. Ultimately, the adopted approach allows the effect of the working-fluid parameters, namely the critical temperature and ideal specific-heat capacity, on both the expander performance and the cycle to be evaluated in a generalised way. For the investigation, 15 theoretical working fluids are defined, covering five different critical temperatures, with a negatively-sloped, vertical and positively-sloped saturated vapour line respectively. The 15 working fluids are selected as they represent the feasible design space occupied by existing ORC working fluids. For each fluid, a cycle optimisation is completed for different heat-source temperatures ranging between 80 and 200 °C. The objective is to identify the optimal cycle operating conditions that result in maximum power output from the system. By analysing the results, the optimal characteristics of a working fluid are obtained, and this information can be used to identify physical working fluids which are good candidates for a particular heat-source temperature. In the final part of this paper, the cycle optimisation is repeated for the physical working fluids identified, thus validating the suitability of the approach developed. Ultimately, the results can help to narrow down the search space when considering working fluids for an ORC operating with two-phase expansion.

1. INTRODUCTION

The organic Rankine cycle (ORC) is widely considered to be a suitable technology for the conversion of low-temperature heat into power. However, due to low heat-source temperatures the conversion efficiency of an ORC system is generally low, while system costs are relatively high, which means high payback periods remain a stumbling block for the technology. Therefore, a large amount of research concerning cycle innovation has been conducted over recent years with a view to identifying systems with improved performance, both from the point of view of thermodynamics and economics.

One idea to improve the performance of ORC systems is to allow the expansion process to occur within the two-phase region, and in the most extreme case from a saturated liquid (Smith, 1993; Fischer, 2011; Read *et al.*, 2017). This idea is of particular interest for waste-heat recovery applications, in which it is advantageous to cool down the heat source down as much as possible since the heat would otherwise be wasted. Therefore, by expanding the working fluid from a two-phase state much of the isothermal heat transfer that would otherwise occur in a conventional ORC can be removed, which allows a much better thermal match between the heat source and working fluid to be achieved, thus leading to less irreversibility in the heat-transfer process and higher power outputs.

From a theoretical perspective, the thermodynamic benefits of operating an ORC with two-phase expansion have been well reported within the literature (Smith, 1993; Fischer, 2011; Read *et al*., 2017). However, the major challenge to successfully achieving two-phase expansion within ORC systems is the identification and development of suitable expander technologies. Existing research activities have focussed on volumetric expanders for two-phase expansion since turbo-expanders are not designed for two-phase conditions at the expander inlet. For power outputs exceeding a few tens of kW, screw expanders can be considered one of the most suitable technologies and have been the subject of previous research activities (Smith *et al.,* 1996; Öhman & Lundqvist, 2013; Bianchi *et al*., 2017; Bianchi *et al*., 2018). Moreover, ORC systems operating with twin-screw expanders are already commercially available in the range of 35 to 110 kW_e (Electratherm, 2015). However, one disadvantage of twin-screw expanders is that the maximum built-in volume ratio of the machine is limited by mechanical design constraints, such as thermal distortion and bearing loads. Therefore, as the volumetric expansion ratio (*i.e.*, the ratio of the fluid density at the inlet and outlet of the expander) increases beyond a certain value, the isentropic efficiency of the expander reduces (Read *et al*., 2014). Therefore, when modelling two-phase expansion within ORC systems it is important to implement a suitable expander model to account for the effect of the expansion volumetric ratio on the expander efficiency.

Another important area of research into ORC systems remains in the identification of optimal working fluids. In particular, the use of computer-aided molecular design (CAMD) methods to simultaneously optimise the working fluid alongside the thermodynamic cycle has recently become more prevalent (Schilling *et al*., 2016; Cignitti *et al*., 2017; White *et al*., 2017). Such methods allow the properties of an optimal working fluid to be studied more generally than would otherwise be possible using programs such as NIST REFPROP (Lemmon *et al*., 2013). However, compared to fluid selection for ORC systems operating with superheated expansion, the identification of optimal fluids for two-phase expansion has not been studied in detail. Moreover, it cannot be immediately assumed that the characteristics that make one fluid the optimal choice for superheated expansion will also mean it is an optimal choice for two-phase expansion.

The aim of this paper is to attempt to study the characteristics of an optimal fluid for ORC systems operating with a twin-screw expander to achieve two-phase expansion. The working fluid is modelled using the Peng-Robinson equation of state, which in turn allows a potential working fluid to be modelled by six adjustable parameters, and the effects of these parameters to be studied. Moreover, a suitable expander performance model is implemented to account for the effect of the expansion volumetric ratio on the overall performance of the system.

2. MODELLING

2.1 Peng-Robinson equation of state

To model the working fluid the Peng-Robinson equation of state is used:

$$p = \frac{RT}{V_\mathrm{m} - b} - \frac{a\alpha(T)}{V_\mathrm{m}^2 + 2bV_\mathrm{m} - b^2}, \tag{1}$$

where p is the pressure in Pa, R is the universal gas constant in J/(mol K), T is the temperature in K and V_m is the molar volume in m^3/mol. The parameters a and b are fluid-specific parameters, which depend on the critical temperature T_cr and critical pressure p_cr of the fluid. The function $\alpha(T)$ introduces a temperature dependence to the term on the right-hand side of Equation 1, and this term is dependent on the acentric factor ω. The full details of these parameters can be found in Poling *et al*. (2001). To be able to compute the single-phase enthalpy h in J/mol, and entropy s in J/(mol K), an expression for the ideal specific-heat capacity is required. This is defined using a second-order polynomial function of the form:

$$c_{p,\mathrm{id}}(T) = c_0 + c_1 T + c_2 T^2, \tag{2}$$

where c_0, c_1 and c_2 are constants for a particular fluid.

The formation described allows a working fluid to be fully defined by six parameters ($T_\mathrm{cr}, p_\mathrm{cr}, \omega, c_0, c_1, c_2$). This formulation means it is possible to study the effects of key fluid parameters, such as the critical temperature, without precisely defining the working fluid. The suitability of this formulation to model working fluids for ORC systems has previously been demonstrated by the authors (White & Sayma, 2018), albeit with single-phase expansion.

2.2 Thermodynamic modelling

An ORC with two-phase expansion can be modelled by three design variables, namely the condensation temperature T_1, the reduced evaporation pressure p_r (p_2/p_{cr} where p_{cr} is the critical pressure) and the expander-inlet vapour quality q_3. The heat-source temperature drop ($T_{\mathrm{hi}} - T_{\mathrm{ho}}$) is an additional design variable which is used to determine the working-fluid mass-flow rate:

$$\dot{m} = \frac{\left(\dot{m}c_p\right)_{\mathrm{h}}(T_{\mathrm{hi}} - T_{\mathrm{ho}})}{h_3 - h_2}, \tag{3}$$

where $\left(\dot{m}c_p\right)_{\mathrm{h}}$ is the heat-source heat-capacity rate in W/K, and h_2 and h_3 are the enthalpies of the working fluid at the inlet and outlet of the evaporator. The heat-source temperature drop is expressed in non-dimensional form:

$$\theta = \frac{T_{\mathrm{hi}} - T_{\mathrm{ho}}}{T_{\mathrm{hi}} - T_{\mathrm{ci}}}, \tag{4}$$

where $T_{\mathrm{hi}}, T_{\mathrm{ho}}$ and T_{ci} are the heat-source inlet temperature, heat-source outlet temperature and heat-sink inlet temperatures respectively.

Alongside these four variables, the pump is modelled by assuming a fixed isentropic efficiency of 70%, and energy balances are applied to the evaporator and condenser to obtain the temperature profiles of the heat source, heat sink and working fluid. These are checked to ensure that imposed minimum evaporator and condenser pinch points, denoted, PP_{h} and PP_{c}, are not violated.

2.3 Twin-screw expander modelling

Following the rationale described in the introduction, it is assumed within this paper that two-phase expansion can be achieved using a twin-screw expander. When considering a particular twin-screw expander for a defined application the two parameters of primary interest are the volumetric expansion ratio $V_{\mathrm{r,exp}}$, and the expander built-in volume ratio $V_{\mathrm{r,bi}}$. The former is defined as the ratio of the fluid densities at the expander inlet and the expander outlet (*i.e.*, ρ_3/ρ_4), whilst the latter is the ratio of the chamber volume at the inlet and outlet of the machine and this is fixed for a given machine.

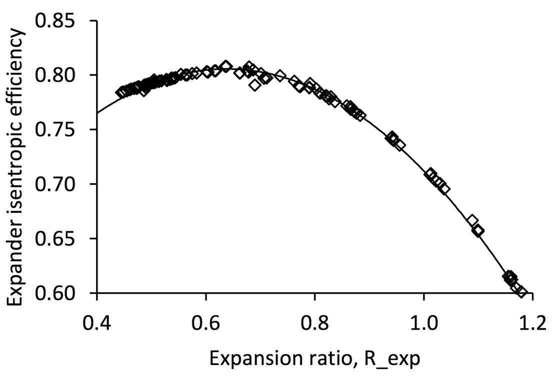

Figure 1: Relationship between the expansion ratio ($R_{\mathrm{exp}} = V_{\mathrm{r,bi}}/V_{\mathrm{r,exp}}$) and the isentropic efficiency of a twin-screw expander (Read *et al.*, 2014).

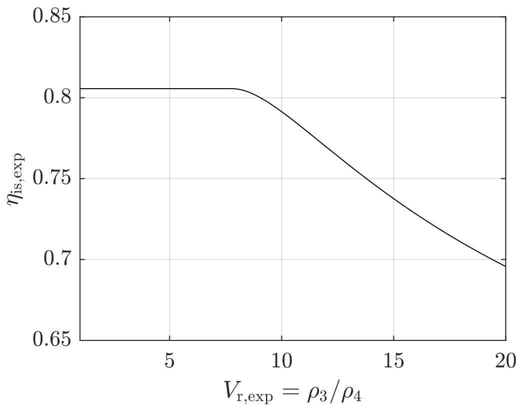

Figure 2: Twin-screw expander isentropic efficiency $\eta_{\mathrm{is,exp}}$ as a function of expansion volume ratio $V_{\mathrm{r,exp}}$, assuming a maximum built-in volume ratio of 5

Previously, Read *et al.* (2014) have shown that the isentropic efficiency of a twin-screw expander is related to the ratio of these volume ratios, defined as $R_{\mathrm{exp}} = V_{\mathrm{r,bi}}/V_{\mathrm{r,exp}}$. This relationship is shown in Figure 1, and it is observed that an optimal expander isentropic efficiency is obtained for $R_{\mathrm{exp}} \cong 0.65$. The maximum built-in volume ratio for a twin-screw expander is limited by mechanical design constraints; as the required built-in volume ratio increases, the length of the rotor required which introduces challenges with regards to thermal distortion and bearing loads. Within this paper, it is assumed that the maximum built-in volume ratio is 5. Therefore, the maximum volumetric expansion ratio that can be achieved using a twin-screw expander, without resulting in a reduction in the expander isentropic efficiency, is 5/0.65 = 7.7. Using this, it is possible to derive an expression for the expander isentropic efficiency as a function of the volumetric expansion ratio. For $V_{\mathrm{r,exp}} \leq 7.7$ it is assumed that a twin-screw expander can be selected, or designed, that has an optimal built-in volume ratio such that $R_{\mathrm{exp}} = 0.65$. For $V_{\mathrm{r,exp}} > 7.7$, the expander isentropic efficiency can be estimated using a second-order polynomial curve fit for the data shown in Figure 1. This is expressed mathematically as follows:

$$\eta_{\mathrm{is,exp}} = \begin{cases} \eta_{\mathrm{is,max}}\,, & V_{\mathrm{r,exp}} \leq 7.7 \\ -0.7205R_{\mathrm{exp}}^2 + 0.9230R_{\mathrm{exp}} + 0.5100\,, & V_{\mathrm{r,exp}} > 7.7 \end{cases} \tag{5}$$

and this correlation is shown graphically in Figure 2 for an assumed maximum built-in volume ratio of 5. Alongside Equation 5, the screw expander is modelled assuming a mechanical efficiency of 90%.

3. CASE STUDY DEFINITION

3.1 Working-fluid definition

Combining the Peng-Robinson equation of state with the thermodynamic and expander models it is possible to investigate the optimal characteristics of working fluid intended for ORC applications operating with two-phase expansion. Following from a previous study conducted by the authors (White & Sayma, 2018), the values for p_{cr} and ω do not have a significant effect on the cycle behaviour, and these are fixed to values of 30 bar and 0.3 respectively. Therefore, the main fluid parameters are the critical temperature and the coefficients for the second-order polynomial that describes the ideal specific-heat capacity.

The variation in the ideal specific-heat capacity with temperature for a range of fluids is shown by the black dotted lines in Figure 3. These lines correspond to typical working fluids for low-temperature ORC systems, and the data has been obtained using NIST REFPROP. Based on this data, three different fluid types can be defined, denoted Fluid A, Fluid B and Fluid C respectively. The coefficients for the ideal specific-heat capacity for these three fluid types are listed in Table 1, and the resulting variation in the ideal specific-heat capacity with temperature is also shown in Figure 3. Ultimately, these three fluids are defined in such a way as to effectively capture the range of behaviour observed for physical working fluids.

Table 1: Ideal specific-heat capacity coefficients for the three different types of fluid

	c_0 [J/(mol K)]	c_1 [J/(mol K^2)]	c_2 [J/(mol K^3)]
Fluid A	10	0.20	1×10^{-4}
Fluid B	30	0.25	1×10^{-4}
Fluid C	20	0.40	1×10^{-4}

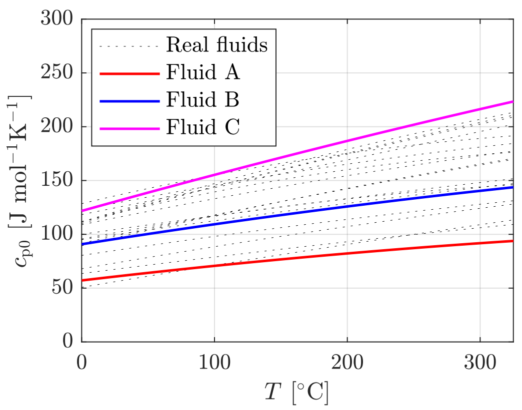

Figure 3: Variation in the ideal specific-heat capacity with temperature for the three fluid types defined (Fluid A, Fluid B and Fluid) in addition to physical working fluids available in REFPROP

Alongside defining the coefficients for the ideal specific-heat capacity polynomial, five different critical temperatures are defined, namely 100, 125, 150, 175 and 200 °C respectively. This results in a total of 15 defined working fluids. The saturation domes for nine of these 15 fluids are shown in Figure 4 (the fluids with T_{cr} = 125 °C and 175 °C are omitted for clarity). As observed in this figure, the coefficients for Fluids A, B and C correspond to working fluids with saturation vapour line that is negatively-sloped, vertical, and positively-sloped respectively; these types of fluids are often termed as being 'wet', 'isentropic' and 'dry' respectively.

3.2 Optimisation setup

For the 15 defined working fluids, an ORC system operating with two-phase expansion can now be optimised, and the characteristics of an optimal working fluids identified. In this paper, the aim of the optimisation is to identify fluids that result in the maximum power output from the system, although other objectives such as minimising specific-investment costs should be considered in future. Therefore, since the fluid parameters are fixed, the optimisation consists of optimising four cycle variables (T_1, p_r, q_3 and θ), subject to the imposed evaporator and condenser pinch points ($PP_h = PP_c = 10$ K). Moreover, the condensation pressure is constrained to avoid sub-atmospheric condensation (*i.e.*, $p_1 \geq 1$ bar). Since this study is focussed on thermodynamic optimisation and working-fluid selection, which are independent of the size of the system, the heat source is defined with an arbitrary heat-capacity rate of $\dot{m}c_p = 1$ kW/K. The heat sink is assumed to be water at a temperature of 15 °C, with a mass-flow rate of 5 kg/s.

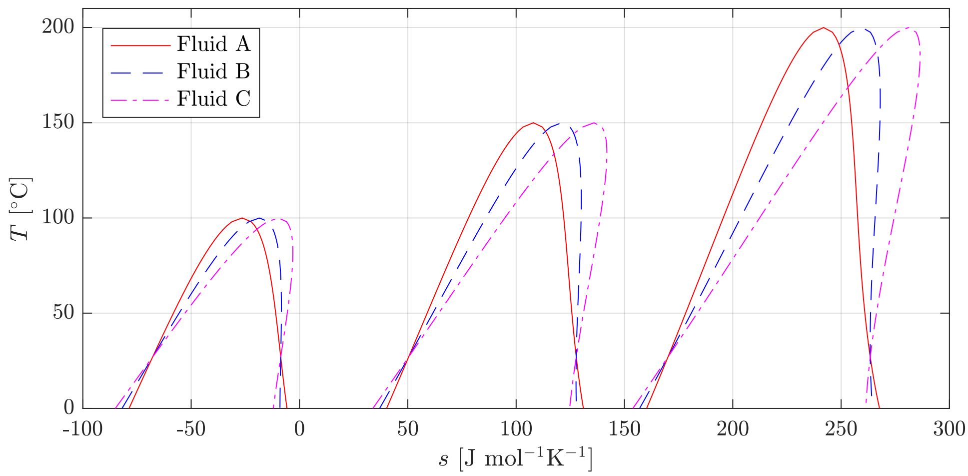

Figure 4: Nine of the 15 defined working fluids shown on a temperature-entropy ($T - s$) diagram

The optimisation is formulated in MATLAB and solved using the sequential-programming algorithm. For each working fluid the optimisation is repeated for four different heat-source temperatures, namely $T_{hi} = 80, 120, 160$ and 200 °C. Moreover, to enable a comparison between theoretically optimal cycles in which the maximum expansion volumetric ratio is unconstrained, and physical cycles in which high expansion volumetric ratios result in a reduced expander efficiency, the optimisation is first conducted for a fixed expander isentropic efficiency (unconstrained) and then repeated using Equation 5 to model the twin-screw expander (constrained).

4. RESULTS

The results from all of the optimisation studies are shown in Figures 5—8, with each figure corresponding to a particular heat-source temperature. In each figure, the results are shown in terms of the optimal net power output $\dot{W}_n$, expander-inlet vapour quality q_3 and expansion volume ratio $V_{r,exp}$ for the 15 working fluids defined in Section 3.1. Moreover, each figure also shows the results for the constrained and unconstrained cases.

Starting first with the results for the 80 °C heat source (Fig. 5), it is observed that Fluid C with a critical temperature of 150 °C results in the maximum net power output for both the constrained and unconstrained cycles, which correspond to 1.82 and 1.86 kW respectively. The percentage reduction $\dot{W}_n$ for the constrained cycle is only 2.1% compared to the unconstrained cycle, although there is a significant reduction in $V_{r,exp}$ from 17.3 to 8.5. Moreover, the constrained cycle results in a higher expander inlet vapour quality (0.083) compared to the unconstrained cycle (0.032). In fact, these observations are found for most of the working fluids, with the exception of the $T_{cr} = 100$ °C fluids, suggesting that constraining the expansion volumetric ratio will generally lead to an optimal system with a higher expander-inlet vapour quality compared to the unconstrained cycle.

Considering the effect of the critical temperature on the optimal cycles (Fig. 5), it is observed that a higher-critical temperature leads to a lower expander-inlet vapour quality, and in the case of the unconstrained cycles a much higher expansion volumetric ratio. The sudden drop in both $\dot{W}_n$ and $V_{r,exp}$ for $T_{cr} = 200$ °C occurs due to the condensation pressure constraint which means it is necessary to increase the condensation temperature to avoid sub-atmospheric condensation pressures. It can therefore be concluded that if the condensation pressure constraint was removed an unconstrained cycle operating with a fluid with T_{cr} = 200 °C would result in an even high-volumetric ratio. It is also interesting to compare the trend in $V_{r,exp}$ as T_{cr} is increased for the different fluid types for the unconstrained cases. Clearly, for a given critical temperature, Fluid C results in the highest expansion volumetric ratio, followed by Fluid B and then Fluid A. This is easily understood by referring to Figure 4 and considering an isentropic expansion from a given evaporation pressure and vapour quality for the three different fluid types. As the gradient of the saturated vapour line becomes more positive, the expander outlet conditions following an isentropic expansion will have a higher vapour quality. Since the density of liquid is much greater than the density of vapour, and a higher vapour quality corresponds to a higher percentage of vapour present within the fluid, it is clear that the more positive the saturated vapour line is, the lower the density of the fluid at the expander outlet, and the higher the expansion volume ratio. With this in mind, one might have expected that for the constrained cases Fluid C would be the least favourable; however, this does not appear to be the case.

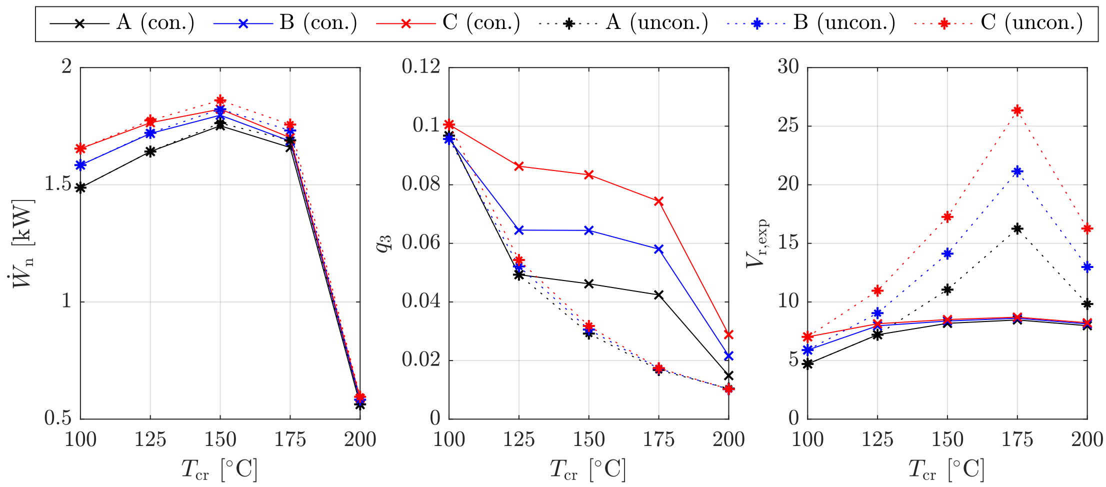

Figure 5: Optimal cycles for Fluid A, B and C with different critical temperatures for T_{hi} = 80 °C. Results are shown in terms of the optimal net power output (left), expander-inlet vapour quality (middle) and expansion volume ratio (right). The constrained (con.) and unconstrained (uncon.) cases refer modelling the expander using Eq. (5) and assuming a constant expander efficiency respectively.

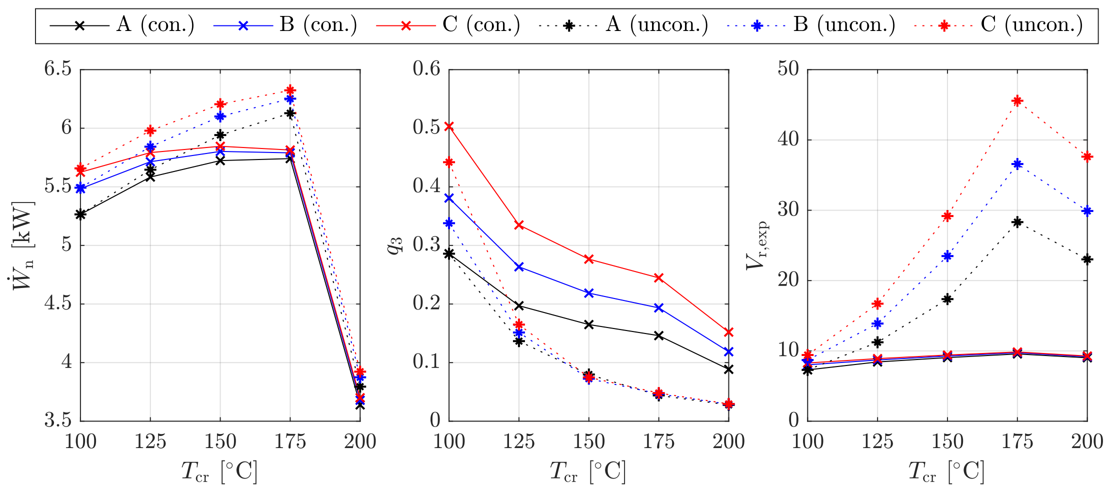

Figure 6: Optimal cycles for Fluid A, B and C with different critical temperatures for T_{hi} = 120 °C. Results are shown in terms of the optimal net power output (left), expander-inlet vapour quality (middle) and expansion volume ratio (right). The constrained (con.) and unconstrained (uncon.) cases refer modelling the expander using Eq. (5) and assuming a constant expander efficiency respectively.

With regards to the remaining heat-source temperatures (Figs. 6—8), many of the same observations are made, with Fluid C generally resulting in the highest power output, higher expander-inlet vapour qualities, and higher expansion volumetric ratios. Moreover, q_3 reduces as T_{cr} increases, and in the case of the unconstrained cycles the optimal volumetric expansion ratio increases until the condensation pressure constraint is violated. When comparing the constrained and unconstrained cycles it is observed that the relative reduction in the power output for the constrained cycles compared to the unconstrained cycles increases as the heat-source temperature increases. This was to be expected since a higher heat-source temperature generally facilitates a higher pressure ratio, and therefore expansion volumetric ratio, and a better thermodynamic performance. However, in the case of the constrained cycles, expansion volumetric ratios above 7.7 are penalised by a reduced expansion efficiency. Moreover, as the critical temperature of the working fluid is increased, and the difference between the unconstrained expansion volumetric ratio and the constrained volumetric expansion ratio increases, the relative reduction in power increases. This may suggest that when considering the limitations of twin-screw expanders, it may not be suitable to select working fluids with higher critical temperatures as the heat-source temperature increases. For example, for the 80 and 120 °C heat sources the constrained cycle that results in the highest power output operates with a fluid with T_{cr} = 150 °C. However, for the 160 °C heat source, the constrained cycle that results in the highest power output operates with a fluid that actually has a lower critical temperature (T_{cr} = 125 °C). This result is contrary to the authors' previous study which showed that for an ORC operating with superheated expansion the critical temperature and heat-source temperature are proportional to each other (White & Sayma, 2018). This demonstrates the role that the expander has on fluid selection, particularly for two-phase expansion.

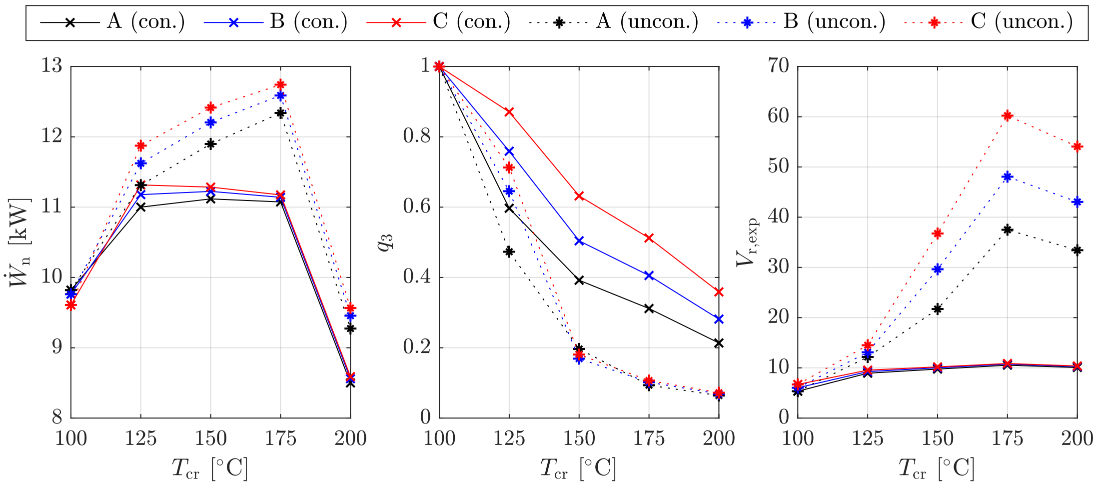

Figure 7: Optimal cycles for Fluid A, B and C with different critical temperatures for T_{hi} = 160 °C. Results are shown in terms of the optimal net power output (left), expander-inlet vapour quality (middle) and expansion volume ratio (right). The constrained (con.) and unconstrained (uncon.) cases refer modelling the expander using Eq. (5) and assuming a constant expander efficiency respectively.

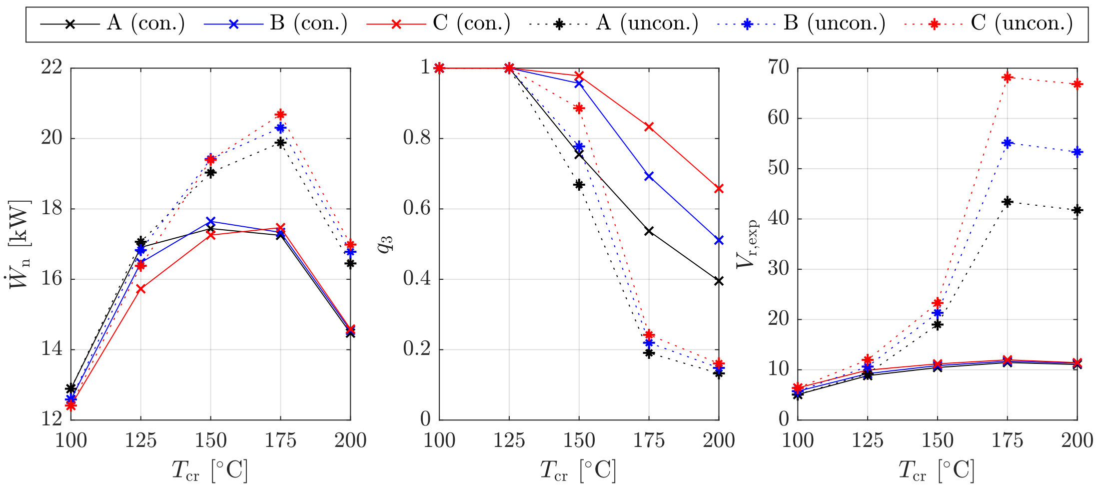

Figure 8: Optimal cycles for Fluid A, B and C with different critical temperatures for T_{hi} = 200 °C. Results are shown in terms of the optimal net power output (left), expander-inlet vapour quality (middle) and expansion volume ratio (right). The constrained (con.) and unconstrained (uncon.) cases refer modelling the expander using Eq. (5) and assuming a constant expander efficiency respectively.

Considering the relationship between the heat-source temperature and the expander-inlet vapour quality as the heat-source temperature increases, it is found that increasing the heat-source temperature will generally result in a cycle with a higher expander-inlet vapour quality. Moreover, for none of the studies was it found that a vapour quality of zero (*i.e.*, a trilateral cycle) resulted in an optimal power output, suggesting there may be some benefit to two-phase expansion compared to expansion from a saturated liquid.

The three fluids that result in the highest net power output for each heat-source temperature are summarised in Table 2. It is found that, with the exception of the third fluid for T_{hi} = 200 °C, there are four working fluids that result in optimal thermodynamic performance, namely Fluid B with T_{cr} = 150 °C and Fluid C with T_{cr} = 125, 150 and 175 °C. This suggests that these four fluids could be broadly suitable for two-phase expansion using twin-screw expanders. Therefore, if physical fluids can be identified that have similar properties to these four theoretical fluids, it stands to reason that good thermodynamic performance can be expected from the cycle.

By inspecting fluids available within the REFPROP program, seven physical working fluids have been identified that have critical temperatures ranging between 134.8 °C (iso-butane) and 196.7 °C (*n*-pentane). The saturation dome for these seven fluids are compared to the saturation dome for the theoretical fluids in Figure 9. Ultimately, it is observed that the four theoretical fluids exhibit similar behaviour to physical working fluids. For each of these physical working fluids, the optimisation of the thermodynamic cycle for each heat-source temperature can be repeated, this time using these defined fluids and using NIST REFPROP to determine the fluid properties. The net power output predicted by these additional optimisations are shown in Figure 10.

Table 2. The three fluids that result in the highest net power output for each heat-source temperature.

Rank	T_{hi} = 80 °C		T_{hi} = 120 °C		T_{hi} = 160 °C		T_{hi} = 200 °C	
	Fluid	T_{cr} [°C]	Fluid	T_{cr} [°C]	Fluid	T_{cr} [°C]	Fluid	T_{cr} [°C]
1	C	150	C	150	C	125	B	150
2	B	150	C	175	C	150	C	175
3	C	125	B	150	B	150	A	150

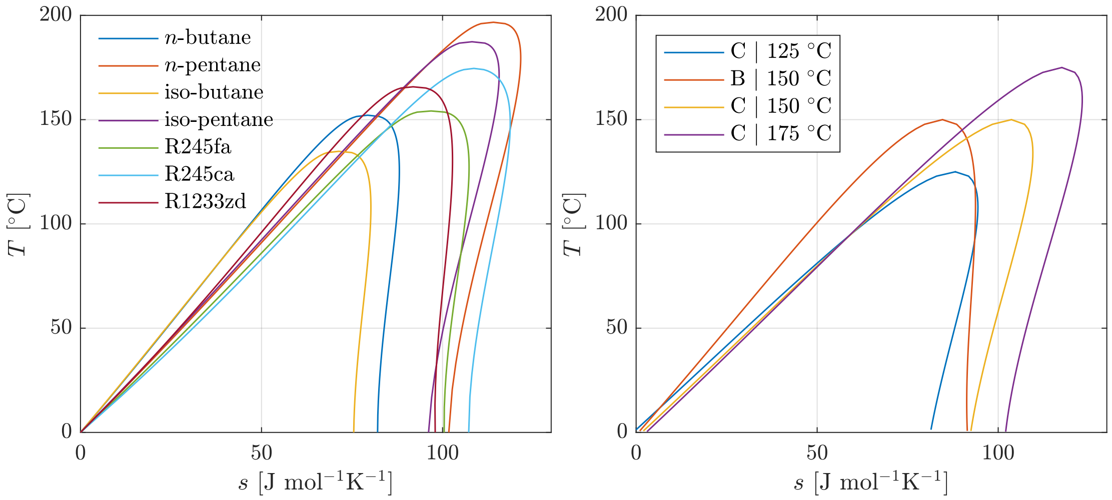

Figure 9: Comparison between the saturation domes for seven physical working fluids (left) and the four theoretical working fluids identified within this study.

From the REFPROP results, it is found that for heat-source temperatures of 80, 120, 160 and 200 °C the optimal fluids are R245ca, iso-pentane, *n*-butane and *n*-butane respectively. The corresponding optimal net power outputs are 1.85, 5.88, 11.41 and 18.08 kW, which are 1.50%, 0.57%, 0.84% and 2.44% higher than the optimal net power outputs obtained using the model developed with the Peng-Robinson equation of state. Comparing the optimal fluids identified from REFPROP, and those identified in Table 2, a reasonable agreement is observed. For example, the results from the Peng-Robinson model would suggest that for heat-source temperatures of 160 and 200 °C either *n*-butane or iso-butane could be a good choice, and this is indeed confirmed by the results obtained using REFPROP. For the lower heat-source temperatures the agreement is not quite as good, as the results using the Peng-Robinson model tend to suggest R245fa is a suitable working fluid, whilst R245ca and iso-pentane are identified as optimal fluids from the REFPROP results. However, the percentage reductions in net power output for R245fa are only 1.33% and 1.27% respectively, indicating that R245fa could still be a suitable choice. Overall, the small differences between the two models confirms that the model, based on the Peng-Robinson equation of state, can be used to identify working fluids for ORC systems operating with two-phase expansion.

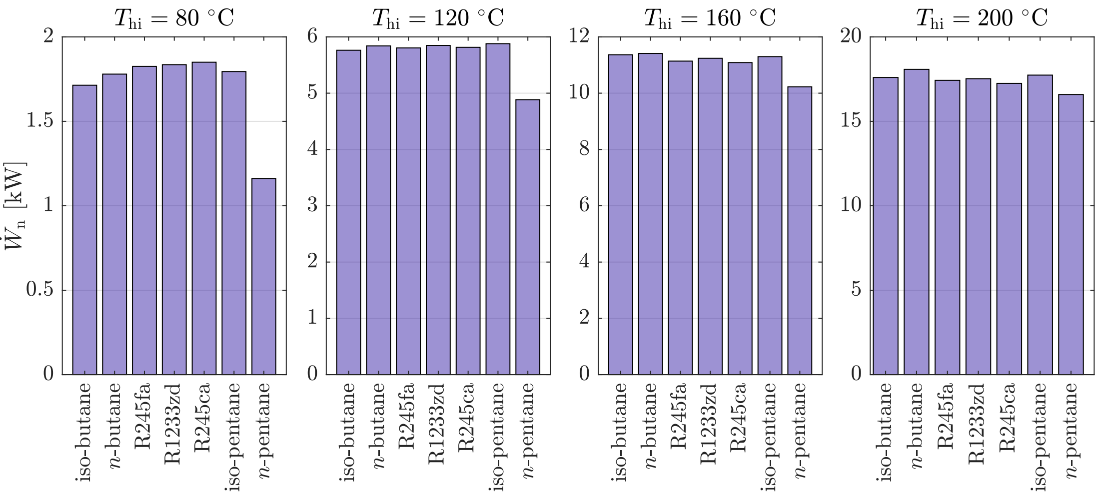

Figure 10: Optimal net power output for ORC systems operating with two-phase expansion for different working fluids. Results are obtained using NIST REFPROP to model the fluid properties. Results are plotted with critical temperature of the working fluid increasing from left to right.

5. CONCLUSIONS

This paper has detailed the development of a methodology to investigate the optimal characteristics of working fluids for ORC systems operating with two-phase expansion using a twin-screw expander. The method is comprised of a thermodynamic system model, the Peng-Robinson equation of state and a simple correlation to account for the effect of the expansion volumetric ratio on the expander isentropic efficiency. After defining 15 theoretical working fluids, an optimisation study was completed for heat-source temperatures ranging between 80 and 200 °C. From the results a number of conclusions can be made. Firstly, for all the cases considered it is found that the optimal expander inlet vapour quality reduces as the critical temperature is increased, but on the whole increases as the heat-source temperature is increased. Moreover, when considering the limitation in the expansion volumetric ratio, imposed by using a twin-screw expander, the optimal expander inlet vapour quality increases further. Secondly, it is observed that for a given heat-source temperature there is an optimal critical temperature at which power output will be obtained. Above this optimum there is a reduction in power output which is caused by increasing the condensation pressure to avoid sub-atmospheric condensation pressures. In general, it is observed that for heat-source temperatures ranging between 80 and 200 °C, the optimal critical temperature ranges between 125 and 175 °C. The results also suggest that there may be a slight thermodynamic benefit in employing a working fluid with a saturated vapour line that has a slightly positive gradient (when viewed on a $T - s$) diagram. Finally, using the results obtained for the theoretical working fluids to identify physical working fluids, it is found that R245ca, iso-pentane and *n*-butane are good candidates for the heat-source temperatures considered.

NOMENCLATURE

a, b	fluid-specific parameters	
c_0, c_1, c_2	ideal specific-heat capacity coefficients	
c_p	specific heat-capacity at constant pressure	(J/(mol K))
$\dot{m}$	mass-flow rate	(kg/s)
p	pressure	(Pa)
p_r	reduced evaporation pressure	
PP_h, PP_c	evaporator and condenser pinch points	(K)
q	vapour quality	
R	universal gas constant	(J/(mol K))
R_{exp}	expansion ratio	
T	temperature	(K)
V_m	molar volume	(m^3/mol)
V_r	volumetric ratio	

$\dot{W}_{\mathrm{n}}$	net power output	(kW)
η_{is}	isentropic efficiency	
θ	non-dimensional heat-source temperature drop	
ρ	density	(kg/m^3)
ω	acentric factor	

Subscripts

1—4	ORC state points
bi	built-in
c	heat-sink (cold)
ci	heat-sink inlet
cr	critical point
exp	expander
h	heat-source (hot)
hi	heat-source inlet
ho	heat-source outlet

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