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(coordinadores)

Proceedings of the 7th International Seminar on ORC Power Systems

Editorial Universidad de Sevilla

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(ORC2023)

4th to 6th
SEPTEMBER
SEVILLE 2023

EDITORIAL UNIVERSIDAD DE SEVILLA

Sevilla, 2024

Colección Actas
Núm.: 91

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ISBN 978-84-472-2745-7
DOI: https://dx.doi.org/10.12795/9788447227457

Diseño de cubierta y maquetación: los autores

INDEX OF CONTRIBUTIONS

DOI: https://dx.doi.org/10.12795/9788447227457_28

Optimization of a Partially Evaporating Organic Rankine Cycle with thermal non-equilibrium expansion.

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ABSTRACT

The Trilateral Flash Cycle (TFC) is an alternative to the Organic Rankine Cycle (ORC). The TFC have been shown to have greater exergy efficiencies compared to the ORC in low-grade heat-to-power conversion. This is a result of the more efficient heat transfer from the heat carrier to the working fluid, even though the TFC has inherently a lower thermal efficiency. However, these results are based on cycle modeling assuming equilibrium conditions, but the actual two-phase expansion process is a non-equilibrium process. Thermal non-equilibrium between vapour and liquid occurs during the evaporation (or flashing) of the working fluid during the two-phase expansion process. The liquid phase has a temperature greater than the corresponding pressure's saturation temperature and the equilibrium assumption overestimates the actual vapour quality. In a previous work, this non-equilibrium expansion was modeled and predicted based on the homogeneous relaxation model (HRM). In this work, the impact of the non-equilibrium process on the efficiency of the TFC is investigated and compared to the equilibrium model. The overall power recuperation is around 86% lower when including the thermal non-equilibrium nature of the expansion process. Therefore, the thermodynamic non-equilibrium losses should thus be incorporated when predicting the performance of a TFC. 176

1 INTRODUCTION

The reduction in greenhouse gas emissions, to reduce the effects of climate change, consists of a wide variety of possible actions. One such action is the reduction of the total process losses through recuperative methods. One of the most significant losses with the current global infrastructure is waste heat (Firth *et al.*, 2019, Forman *et al.*, 2016) for which there exist multiple methods to recover this lost energy. The estimated global waste heat is around 52% of the global energy input of which around 65% is low-temperature waste heat. If these waste energy streams could be efficiently harvested, it would reduce the required initial energy input as a larger share of this energy would become useful, reducing greenhouse gas emissions in the process. The largest untapped sector of waste heat was the transport sector according to Firth *et al.* (2019). Methodologies to harvest waste heat exist such as the Organic Rankine Cycle (ORC) or variants thereof. One such variant is the Trilateral Flash cycle (TFC) which does not evaporate the working fluid in the evaporator. Instead, a saturated liquid is expanded to the low pressure compared to a superheated vapour in the basic ORC. This cycle has larger net power output compared to the basic ORC (Li *et al.*, 2017, Fischer, 2011), especially with lower heat source temperatures (Woodland *et al.*, 2020). This is a result of the better temperature profile matching between the waste heat carrier and the working fluid (Lecompte *et al.*, 2015a) within the evaporator. However, these studies do assume similar isentropic efficiencies for both vapour and two-phase expanders. It is also possible to partially evaporate the working fluid within the evaporator of the cycle, this cycle is known as the Partially Evaporating Organic Rankine Cycle (PEORC). This reduces the temperature profile matching but also decreases the volume flow rate of the cycle compared to the TFC, which can become large (Fischer, 2011). This can result in higher net power output of the cycle (Lecompte *et al.*, 2013) due to the reduction in required pumping power. This is especially the case when the pump's isentropic efficiency is low.

In literature, when cycles are studied which incorporate two-phase expansion, assumptions are made to describe this process. As mentioned, it is often based upon an isentropic efficiency, as similarly done for vapour expansion processes. Another assumption often made is the thermodynamic stability of the process. However, it has been shown that this assumption does, depending on the expander type, not have good agreement with experimental data. Currently, this assumption corresponds to experimental data for Lysholm expanders operating in two-phase conditions (Öhman and Lundqvist, 2013) but not for reciprocating expanders (Kanno and Shikazono, 2015) where the non-equilibrium effects are not negligible and represent a substantial part of the losses.

In previous work (van Heule *et al.*, 2023), the two-phase expansion within a reciprocating expander was modelled by using an adapted homogeneous relaxation model (HRM) and compared to the homogeneous equilibrium model (HEM). The HEM is based on the conservation equations with the assumption that the mixture is in thermodynamic equilibrium at all times. This implies that evaporation can happen instantaneously. The HRM is based on the HEM but without the thermal equilibrium assumption. Instead, a vapour generation rate equation is used which describes the evaporation rate based on a relaxation equation (Downar-Zapolski *et al.*, 1996). Hereby it is possible to have a mixture of saturated vapour and superheated liquid at the same chamber pressure as was also experimentally observed by Kanno and Shikazono (2015). In this work, this model is implemented within a Trilateral Flash cycle and optimized based on the cycle's net power output which is compared to an optimization with the HEM expansion.

2 METHODS

2.1 Modeling of thermal non-equilibrium expansion

The thermal non-equilibrium occurring within the expander chamber of a reciprocating expander was chosen to be modelled with an adapted Homogeneous Relaxation Model. This model assumes that the phases have the same pressure, as they occupy the same expansion volume, but not that the phases necessarily have the same temperature even though the expansion occurs within the two-phase region. This is a result of an evaporation equation that limits the evaporation rate through an empirical thermal relaxation time as expressed in equations (1) and (2):

$$\frac{\Gamma_g}{\rho} = -\frac{x - \bar{x}}{\Theta} \tag{1}$$

$$\Theta = \Theta_0 \cdot \epsilon^a \cdot \psi^b \tag{2}$$

, where Γ_g is the volumetric vapour generation rate, ρ the mixture density, x the actual vapour quality, $\bar{x}$ the equilibrium vapour quality, Θ the relaxation time, ϵ the void fraction and ψ the non-dimensional pressure difference defined in equations (3) and (4) depending on the operational pressure.

$$\psi = \frac{p_s - p}{p_s} \qquad if\ p < p_{\lim} \tag{3}$$

$$\psi = \frac{p_s - p}{p_c - p_s} \qquad if\ p > p_{\lim} \tag{4}$$

where p_s is the saturation pressure corresponding to the liquid superheat, p is the actual pressure, p_c is the critical pressure, and $p_{\lim}$ an empirical pressure threshold. The values of the numerical parameters Θ_0, a, and b in equation (2), determined experimentally by Downar-Zapolski *et al.* (1996), are respectively $6.51 * 10^{-4} s$, -0.257 and -2.24 when equation (3) is used and $3.84 * 10^{-7} s$, -0.54 and -

1.76 when equation (4) is used and the empirical pressure threshold was 10 bar. These values were based on water flowing through a diverging nozzle. This was adapted by van Heule *et al.* (2023) based on the experimental data of Kanno and Shikazono (2017) who performed expansion experiments with water in a piston moving with a trapezoidal movement profile. Based on this experimental data, the best fitting values of the numerical parameters Θ_0, a, and b are $9 * 10^{-15}s$, -0.7, and -15.7 respectively but only for the definition using equation (3) as only pressures beneath 10 bar were experimented on.

The model keeps track of the mass and internal energy of each phase separately throughout the expansion process. The actual vapour quality can easily be calculated in each time step based on the masses of each phase as expressed in equation (5), while the equilibrium vapour fraction is a function of the total internal energy of the mixture within the expansion chamber and the saturated specific internal energy values corresponding with the chamber pressure as expressed in equation (6):

$$x = \frac{m_g}{m_l + m_g} \tag{5}$$

$$\bar{x} = \frac{u - u_l}{u_g - u_l} \tag{6}$$

where m_g is the vapour mass, m_l the liquid mass, u_g and u_l the specific internal energy of saturated vapour and liquid at the working chamber respectively, and u the specific internal energy of the entire mixture. All fluid properties are obtained through the REFPROP 10 (Lemmon *et al.*, 2018) library including the metastable liquid temperature, required for p_s in equations (3) and (4), based on thespecific internal energy of the liquid phase and the working chamber pressure. The working chamber pressure in turn is obtained through the saturated vapour phase assumption of the HRM model through REFPROP.

2.2 Partial evaporating organic Rankine cycle

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As mentioned in Section 1, the Partial Evaporating ORC (PEORC) is similar to a basic ORC but the working fluid is not fully evaporated within the evaporator. The PEORC used in this study is for a constant heat carrier flow, reciprocating expander geometry, condensing pressure, and evaporating pressure. The boundary conditions used are listed in Table 1 and Figure 1 is an example of the cycle with a vapour quality of 0.3. Point 1 on this figure is determined by the pump subcooling and the condensing pressure. Point 2 is calculated based on constant isentropic pump efficiency. Point 3, the inlet of the expander, is determined by the evaporating pressure and the initial vapour quality of the expansion. Point 4* is the state at the end of the expansion stroke and model. However, this point is not yet in equilibrium and does therefore not have a defined location within this type of temperature-entropy diagram. Here it is plotted on the location with the same density and specific internal energy. The process from point 4* to 4 on Figure 1 is an isochoric process between the metastable point 4* and thermodynamic stable point 4 at the low pressure. This thus includes both non-equilibrium losses and over- or under-expansion losses. Lastly, an isobaric heat rejection process occurs within the condensor to the predefined subcooling to close the cycle. The pinch point condition within the evaporator can occur either at the heat source exit or within the evaporator where the working fluid starts boiling. Which condition occurs depends on the vapour quality at which expansion is occurring. For low vapour qualities at the expander inlet, the pinch point will occur at the heat source outlet, while it occurs at the working fluid saturated point for higher expander vapour qualities. The cycle can dynamically switch between the two conditions depending on which assumed location indeed gives a higher temperature difference at the other location. The geometric properties of the free piston expander are also listed in Table 1 and are based on a reciprocating expander for waste heat recovery of a truck engine (Rijpkema *et al.*, 2021). The stroke and expander cycle speed can be altered based on the requirements of the mass flow rate coupled with the choice of expansion inlet quality. The intake stroke is taken as 25% of the entire expanding stroke (Glavatskaya *et al.*, 2012).

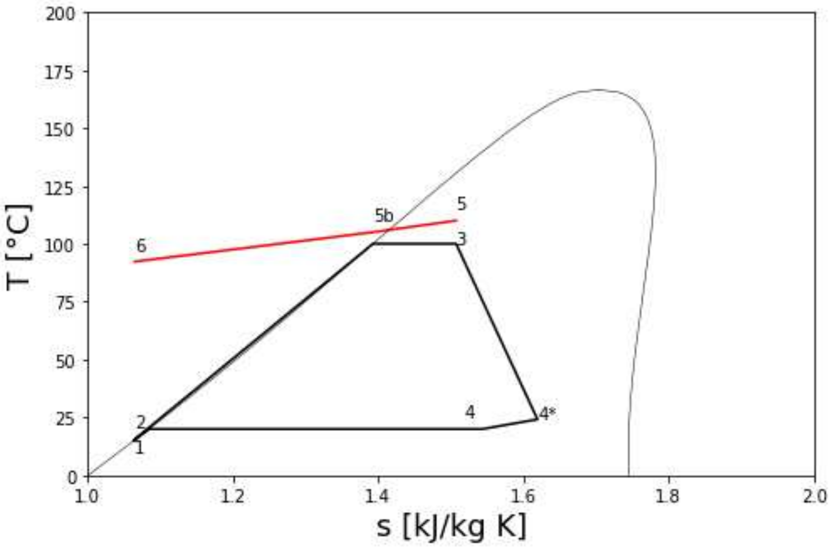

Figure 1: TS diagram of PEORC with expander inlet vapour quality equal to 0.3 where point 4* represents a metastable condition with corresponding density and specific internal energy.

Table 1: Boundary conditions of the partially evaporating Organic Rankine Cycle.

Condensing temperature	20 °C
Evaporating temperature	100 °C
Working fluid	R1233ZD(E)
Heat carrier	Air
Heat source temperature	110 °C
Heat source flow rate	0.2 kg/s
Subcooling pump	5 °C
Evaporator pinch point	5 °C
Isentropic pump efficiency	0.7
Vapour quality at expander inlet	0-1
Expander diameter	0.09 m
Expander clearance length	0.003 m
Intake stroke duration	25 %

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In the following, the cycles will be compared based upon the net power output as defined in equations (7) to (9):

$$W_{net} = W_{exp} - W_{pump} \tag{7}$$
$$W_{pump} = \dot{m_{wf}} \cdot (h_2 - h_1) \tag{8}$$
$$W_{exp} = \frac{\int p \cdot dV}{t_{cycle}} \tag{9}$$

where W_{net} is the net power output of the cycle, W_{exp} the power delivered by the expander during the expansion stroke, W_{pump} the power required to run the pump, $\dot{m_{wf}}$ the mass flow rate of the working fluid, h_2 and h_1 the specific enthalpy at the outlet and inlet of the pump respectively, p the pressure within the working chamber, V the volume of the working chamber, and t_{cycle} the duration of one expander stroke cycle. Because the heat source is taken constant, this power is also a measure of the second law efficiency as defined in equation (10) (Lecompte *et al.*, 2015b):

$$\eta_{II} = \frac{W_{net}}{E_{hs,in}} \tag{10}$$

where η_{II} is the second law efficiency and $E_{hs,in}$ is the exergy flow within the system of the heat source. The isentropic efficiency of the expander is defined in equation (11) were h_3 is the specific enthalpy at the expander inlet (point 3 in Figure 1) and h_{4s}^* the isentropic specific enthalpy of point h_4^* in Figure 1.

$$\eta_s = \frac{W_{exp}}{\dot{m_{wf}} \cdot (h_3 - h_{4s}^*)} \tag{11}$$

3 RESULTS

3.1 Impact of vapour quality on working fluid flowrate

The choice of vapour quality at the start of expansion has a large impact on the required flow rate of the working fluid as presented in Figure 2.

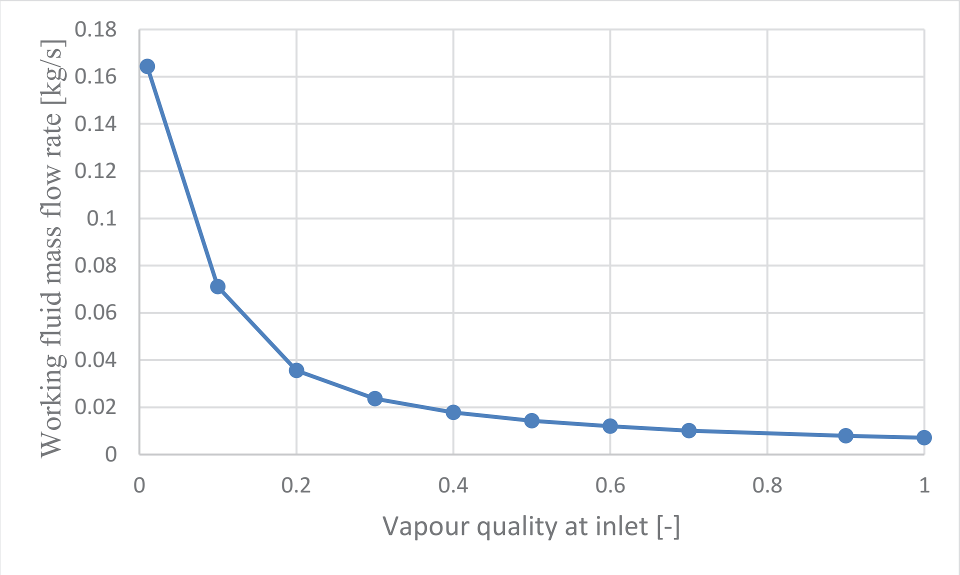

Figure 2: Required working fluid mass flow rate in function of vapour quality.

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As mentioned, this phenomenon of large flow rates is a known issue with the TFC as the required pumping power drastically increases. Choosing a vapour quality already slightly higher than saturated liquid already drastically reduces the required pumping power and thus increases the net power output of the cycle. The difference in the required mass flow rate is also problematic for the chosen expander as the dimensions were predefined. One possibility would be to use multiple expanders and assume the two phase inlet condition is equally split across the different expanders. As an example, using two of these expanders for an inlet vapour quality of 0.1 increases the net power output compared to only one expander as each expander only has half the required mass flow rate resulting in less under expansion losses. However, this does not result in a higher overall net power production compared to other vapour qualities operating with one expander. Thus in the following discussion, only one expander is used irrespective of the vapour quality to find the optimal operation point.

3.2 Cycle optimization

First, the cycle from Table 1 will be optimized for the net power production, defined in Equation (7), with respect to the vapour quality at the end of the evaporator, point 3 in Figure 1. For this configuration, the optimal vapour quality is found to be 0.51 with a net power production of 477.9 W. The net power production in function of vapour quality is shown in Figure 3 where the expanders strokes per minute are optimized on each operation point. A lower vapour quality of the optimum is not beneficial to the cycle as the increase in pumping power is dominant, while an increase in vapour quality is not beneficial due to a reduced heat transfer within the evaporator as a result from the pinch point condition, resulting in less net power production. The optimum point found matches with the speed where the expander on which the dimensions are based (Rijpkema *et al.*, 2021) has an isentropic filling factor of 1. This indicates the important impact of the expander design choice on the optimum working point of the cycle. The isentropic efficiency of the expansion (equation (11)) is also included in Figure 3. This is rather constant around the optimum design point. The impact of the dimensions of the expander on the required strokes per minute and net power is presented in Table 2. A change in the clearance length of the dead volume or the diameter has an impact on the net power but a respectively big change in optimal strokes per minute. The optimum with these other expander dimensions changes for the same cycle.

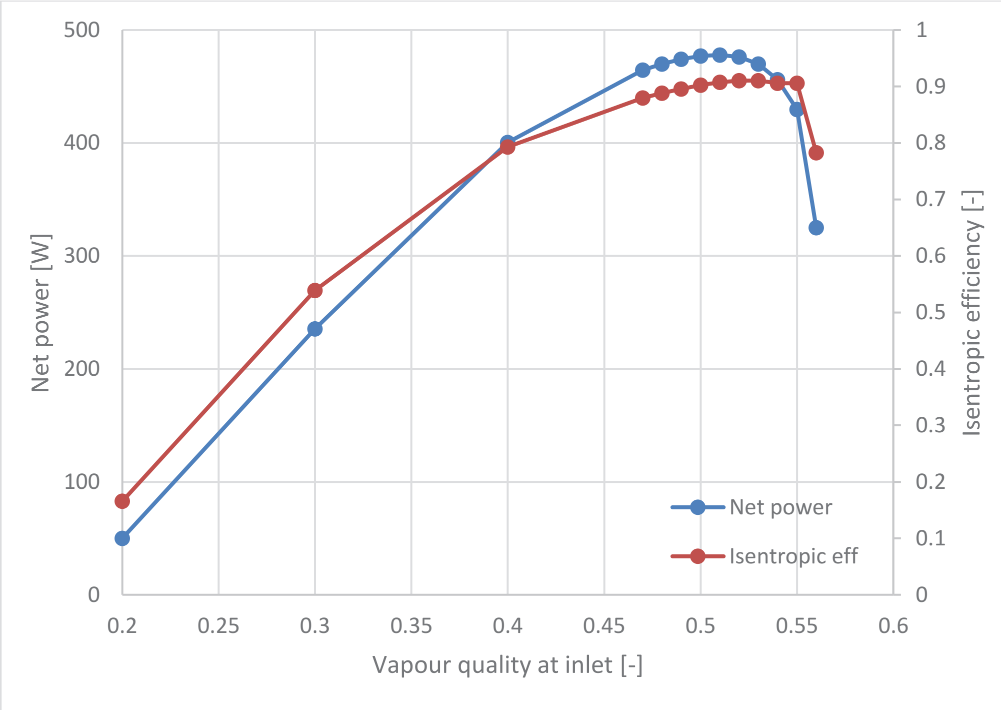

Figure 3: Net power produced of the described TFC in function of vapour quality.

Table 2: Impact of expander dimensions on cycle performance with an expander inlet vapour quality of 0.5.

Diameter [m]	Clearance length [m]	Required strokes per minute [rpm]	Net power [W]
0.09	0.003	963	477.0
0.09	0.002	1575	463.4
0.09	0.004	667	468.0
0.08	0.003	1394	429.9
0.10	0.003	634	459.1

4 DISCUSSION

The performance of the PEORC around the found optimum is compared to the same cycle, but the expansion is modeled without the HRM. It is thus assumed that equilibrium is achieved throughout the entire process at each point in time. The results are shown in Table 3. Firstly the net power with the incorporation of the homogeneous relaxation model is consistently around 86% of the net power output without the HRM which is a non-negligible amount that should be taken into account in cycle comparisons. However, this is less than the benefit gained when comparing the PEORC to a Basic ORC.

It is hereby speculated that the PEORC is still beneficial compared to the Basic ORC for low-temperature heat sources, but in a lesser extent than originally derived. The optimum for the cycle, without incorporating the non-equilibrium expansion, occurs at a slightly lower vapour quality compared to the cycle including the HRM.

Table 3: Cycle performance with HRM and HEM expansion using the same cycle time.

Vapour quality [-]	Net power HRM [W]	Net power HEM [W]
0.54	456.0	526.1
0.53	470.0	543.3
0.52	476.1	551.8
0.51	477.9	555.1
0.50	477.0	555.5
0.49	474.2	553.7
0.48	470.0	550.5

5 CONCLUSIONS

A Trilateral Flash Cycle (TFC) is modeled for a constant heat source, expander design, high pressure, and low pressure. The expansion within the TFC incorporates the thermal non-equilibrium phenomena occurring within a reciprocating expander. This is incorporated through the use of the Homogeneous Relaxation Model (HRM) where the liquid phase can be in a metastable superheated state as the evaporation occurs slower than thermodynamic stable conditions would require. The mass flow rate of the working fluid is heavily dependent on the vapour quality at the evaporator outlet, resulting in very high pumping power for low vapour qualities and thus a low net power output. On the other hand, a decrease in transferred heat within the evaporator for increasing vapour qualities also results in lower net power outputs. Thus an optimum occurs for the chosen cycle and expander. With the choices taken in this paper, the optimum was found at a vapour quality of 0.51. The performance of the chosen cycle is only around 86% of the same cycle when the non-equilibrium expansion is not incorporated within the expander model, indicating the importance of this phenomenon within the reciprocating expander.

In future work, the findings will be validated based on an experimental campaign on a two-phase reciprocating piston expander, which is currently under construction. Additionally, the cycle simulation could be adapted to optimize the cycle without predefining the expander dimensions. In this way, an expander can be designed to best fit a certain application.

NOMENCLATURE

ϵ	void fraction	(–)	ρ	density	(kg/m^3)
Θ	relaxation time	(s)	h	specific enthalpy	(J/kg)
m	mass	(kg)	p	pressure	(Pa)
t	time	(s)	V	volume	(m^3)
u	specific internal energy	(J/kg)	W	power	(W)
$\bar{x}$	equilibrium vapour quality	(–)	x	vapour quality	(–)
Γ	volumetric vapour generation rate	(kg/m^{3}s)			

Subscript

c	critical
g	vapour phase
l	liquid phase
s	saturated
wf	working fluid

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ACKNOWLEDGEMENT

I would like to thank the Research Foundation-Flanders for their financial support through FWO-Flanders grants (1SD9723N).

This book contains the compilation of works contributed to the *7th International Seminar on Organic Rankine Cycle Power Systems* (ORC 2023), held in Seville between the 4th and 6th of September 2023. The event was hosted by Universidad de Sevilla on behalf of the Knowledge Centre on Organic Rankine Cycle Technology (KCORC), incorporated in The Netherlands.

The ORC conference, organized biennially, stems as the only conference that is specific to ORC technology, therefore gathering a diverse community whose affiliation spans across all the interested stakeholders, not only in this particular technology but also and in a broader context, in the energy transition. Original equipment manufacturers, professional associations, end-users, investors, policy makers, academics, scientists feel at home at ORC 2023.

The almost 100 proceedings in this book cover a wide variety of topics, from fundamentals to system integration through component design, accounting for thermodynamic performance as well as component design. In addition to this, and as a new track in 2023, works on heat pump technology were also accepted in order to raise awareness of the strong ties between both technologies, specifically in energy storage applications.

This book provides an excellent overview of the current maturity of power systems based on Organic Rankine Cycle technology for applications as diverse as geothermal and waste heat recovery in industry or downstream of other prime movers (e.g., marine applications). It is also an excellent source of information to understand the current challenges faced by the technology, stemming from a very competitive market and increasingly stringent environmental regulations.

The organizers of ORC 2023 hope that the reader finds this work as exciting as the attendees to the conference and, maybe, make the decision to join the 8th edition to the conference in 2025.

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