David Tomás Sánchez Martínez
Lourdes García Rodríguez
(coordinadores)

Proceedings of the 7th International Seminar on ORC Power Systems

Editorial Universidad de Sevilla

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INDEX OF CONTRIBUTIONS

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Selection of The Optimal Working Fluid in an Organic Rankine Cycle for Waste Heat Recovery Through Multi-Objective Optimization and Decision Making

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ABSTRACT

In India, utilising low-temperature waste heat is crucial to improving energy efficiency. The regenerative organic Rankine cycle (ORC) process is a promising waste heat recovery technique in this study. Here, the thermodynamic behaviour of eight working fluids: Butane, Heptane, Hexane, Pentane, Cyclopentane, HexMDiSiloxn (MM), Benzene, and Toluene, was carefully examined. An elite Non-dominated sorting genetic sorting algorithm (NSGA-II) was used in Multi-objective Optimization (MOO) to address the incongruent behaviour of thermodynamic performance (exergy efficiency) and economic performance (levelized energy cost, LEC). Every eight working fluids are the subject of MOO studies, and the resulting Pareto optimal fronts are created. Several advanced Pareto ranking techniques are taken into account to choose one ideal solution from the Pareto optimal front. These include Simple additive weighting (SAW), The technique for order of preference by similarity to deal Solution (TOPSIS), Grey relation analysis (GRA), and Multi-attributive border approximation area comparison (MABAC).

The most economically advantageous working fluid is chosen using an explicit economic performance assessment index called the Static Investment Payback Period (SIPP). The results show that Pentane is the most economically advantageous working fluid with the shortest SIPP and a medium waste heat temperature range. The findings also imply that any working fluid can be used TOPSIS, SAW, GRA, and MABAC with entropy information considered in this study to recover low-temperature waste heat in the ORC.

1 INTRODUCTION

One of today's most talked-about topics is waste heat recovery. There is always enough waste heat in industrial processes to be directly released into the atmosphere, causing environmental pollution. One of the most important concerns for researchers is how to sustainably reuse or recycle waste heat. Increasing energy consumption and lowering carbon dioxide emissions are crucial to addressing energy and environmental issues (García-Afonso et al., 2022). The organic Rankine cycle (ORC) is the most well-established mechanism in the world for converting waste heat into electricity. The simple, stable, and adaptable ORC technology may recover medium-to-low temperature waste heat (100°C–300°C) (Krishna and Basab 2016).

In an ORC system, heat source temperature, working fluid choice, heat sink conditions, cycle configuration, component selection, and process factors all have an impact on ORC performance (van Kleef et al., 2019). Yet, the primary objective of ORC research has been system optimisation, which is essential for achieving optimal system performance, including selecting the optimal system parameters and working fluid based on waste heat. The most useful optimisation criteria include economic factors like payback period and total investment cost and thermodynamic criteria like thermal efficiency, net power output, etc. (Zhang et al. 2018). Multi-objective Optimisation (MOO) is one of the most effective optimisation techniques for handling this problem with many conflicting objectives. MOO offers a number of solutions that all work just as well in terms of the stated goals. These solutions, which are called Pareto optimal front and nondominated solutions, show how different implementation options and goals affect each other.

In scientific literature, much has been talked about choosing the best solution from a set of nondominated options. Choose one of the non-dominant Pareto-optimal solutions as the next step. There are a number of Pareto-optimal strategies accessible in the literature, with TOPSIS being one of the most popular selection techniques in process engineering. In spite of the fact that finding Pareto-optimal solutions is not yet prevalent in process engineering, there is a great deal of research on the topic. For finding Pareto-optimal solutions, GRA, SAW, CODAS, MEW, MWRA, VIKOR, and MABAC are utilised in addition to TOPSIS (Wang and Rangaiah 2017).

Numerous studies have been conducted based on multi-objective optimisation between optimum thermal efficiency and economic factors. The Levelised Energy Cost with the maximum power output of the ORC system was examined by (Saha et al. 2019). To find the optimal working fluid, they collected waste heat data from five different energy-intensive industries and contrasted maximum exergy efficiency with economical cost using eight different working fluids.

The main goal of this work is to use and compare different ways to find a nondominated solution for applications of regenerative ORC systems. Four methods are chosen for this purpose based on how easy they are to use, how well they can handle goals with different sizes, and how much user input they need. They are implemented using Visual Basic for Applications (VBA) programming in Microsoft Excel.

In addition, a thorough analysis of the thermodynamic analysis and off-design performance of the Regenerative ORC cycle is presented. A Python-based code for thermodynamic cycle simulation has been developed and integrated with the CoolProp fluid properties database. Due to their low global warming potential and ozone depletion potential, eight distinct organic fluids, including Butane, propane, and n-pentane, are considered the working fluids of the Regenerative ORC cycle. Their effect on thermodynamic performance is then evaluated. The most efficient working fluid for cycle configurations is propane.

2 SYSTEM DESCRIPTION

It is imperative to provide a clear and concise account of all materials and methods utilised in the research. This study aims to examine the techniques utilised to enhance the regenerative Organic Rankine Cycle (ORC) efficiency in the context of industrial exhaust gases. Figure 1 below illustrates the schematic depiction of the regenerative ORC. The presented regenerative Organic Rankine Cycle (ORC) is designed to optimise energy recuperation from the available heat sources.

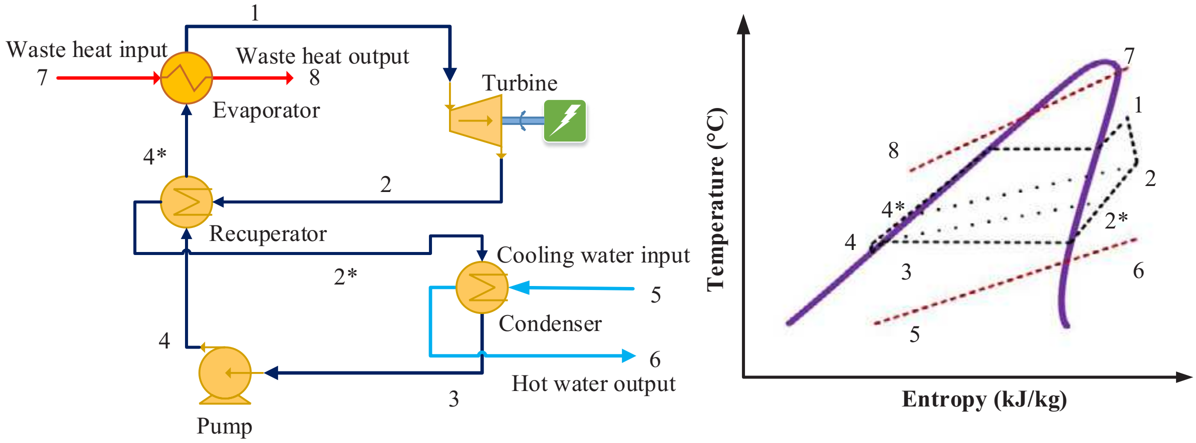


Figure 1: Biaxial machine with the chosen sample geometry

The Regenerative ORC system comprises five distinct equipment components. The components include the evaporator, turbine, recuperator, condenser, and pump. A recuperator is employed in this system to effectively recover the highest amount of thermal energy from the turbine's exhaust. The initial stage of the process involves the utilisation of a pump (process 3-4) to elevate the pressure of the working fluid. Subsequently, the working fluid extracts heat from the recuperator through processes 2-2* and 4-4*. Additionally, the partially heated fluid undergoes a phase change in the evaporator via process 4*-1, utilising waste heat (process 7-8). The fluid characterised by high pressure and temperature undergoes a thermodynamic process (1-2) by entering the turbine and subsequently generating power. The working fluid that has undergone expansion proceeds towards the condenser (through processes 2* -3 and 5-6) to release heat.

2.1 Working fluid selection.

Two crucial evaluation criteria for the ORC system are the Normal Boiling Point (NBP) temperature and the Critical temperature (T_C) of working fluids. Working fluids must also have a high decomposition temperature and stability to prevent flammability, chemical deterioration, non-explosive nature, and non-toxicity. This study also examines the waste heat temperature ranges for choosing the working fluid (see Table 1). This research exclusively considers hydrocarbon-based working fluids. The authors are aware that fluids containing hydrocarbons are combustible. The amount of oxygen a specific hydrocarbon needs to keep a flame is called the minimum combustion oxygen. When oxygen levels fall below this threshold, but hydrocarbon concentrations remain high, and an ignition source is present, deflagration or fire has not occurred. The minimum oxygen content for hydrocarbon combustion ranges from 8 to 12 % by volume. Inflammable hydrocarbon gas concentrations must fall within a specific range. The lower flammability limit is the lowest point in this flammability range (LFL). The upper limit of the range is determined by the Upper Flammability Limit (UFL) (Haq 2021).

Table 1. Selected working fluid for study (Haq 2021).

Working fluids	Molar mass (gm)	T_c	P_c	Safety data		Environmental data			T_w
		°C	bar	LFL (%)	ASHRAE 34 Safety Group	Atmospheric life (Days)	ODP	GWP 100 year	
Benzene	78.1	289	49.0	-	A2	9.4	0		250-300
Butane	58.12	146.1	40.1	-	-	-	0	-	125-200
Cyclopentane	70.1	238	45.8	-	-	-	0		200-275
Heptane	100.2	267	27.3	-	-	-	0	-	225-300
Hexane	86.17	234.6	30.3	-	-	-	0	-	200-275
HexMDiSiloxn (MM)	162.4	245	19.3	-	-	-	0		200-275
Pentane	72.15	196.6	33.7	1.4	-	0.01	0	~20	200-275
Toluene	91.14	318.6	41.2	-	A2	1.9	0	-	275-300

2.2 Description of Thermodynamic Code

To perform a simulation of thermodynamic cycles, an in-house code has been developed to study the impacts of the operating variables. The Python environment has been integrated with the CoolProp database to enable runtime simulation with the available data. The Regenerative ORC cycle has been simulated with a nested iteration of four variables where each single operation parameter has been independently varied over the code execution.

2.3 Mathematical model

The following equation is used to determine the exergy of a stream:

$$\dot{E}x_{mass} = \dot{m}[(h - h_0) - T_0(s - s_0)] \quad (1)$$

The Regenerative ORC cycle's exergy efficiency (EXE) is defined as

$$\eta_{ex} = \left(\frac{W_{net}}{\dot{m}[(h_{W,in} - h_0) - T_0(s_{W,out} - s_0)]}\right) * 100 \quad (2)$$

2.4 Financial Analysis

In this part, the economic model of Regenerative ORC is discussed. The maintenance, operation, and investment costs of Regenerative ORC have been calculated. Also assessed is the projected cost of equipment for the Regenerative ORC. This technique for cost estimation is already discussed in the literature and is acceptable in process engineering. Assume that the heat exchanger, recuperator, and condenser have been constructed from carbon steel and copper. The pump and expander have been constructed from carbon steel (Zhang et al. 2018).

The Bare module cost (C_{BM}) of the Regenerative ORC major component is shown below:

$$C_{BM} = C_{PC}.F_{BM} \quad (3)$$

Here, C_{PC} indicates the purchase cost of the Regenerative ORC component, and the Bare module cost factor of equipment denotes F_{BM}. The Bare module cost factor is dependent on the equipment of the materials.

Purchase equipment cost (C_{PC}) is stated as follows:

$$log_{10}C_{PC} = K_1 + K_2 log_{10}Y + K_3[log_{10}(Y)^2] \quad (4)$$

Where Y is the equipment's capacity or size, the value cost coefficients K_1, K_2, and K_3 are given in Table 2.

The overall amount of capital costs (C_{CC}) is as follows:

$$C_{CC} = \sum C_{BM} \quad (5)$$

The "Chemical Engineering Plant Cost Index (ICEPC)" is added to adjust for inflation-related concerns (Mignard 2014). As reported by equipment manufacturers, the ICEPC values for 2001 and 2022 are 394.3 and 813.0, correspondingly.

All equipment's total capital cost is determined as follows:

$$C_{CC,2022} = \frac{C_{CC}.I_{CEPC,2022}}{I_{CEPC,2001}} \quad (6)$$

The "Capital Recovery Factor (C_{RF})" is computed as follows:

$$C_{RF} = \frac{i(1+i)^n}{(1+i)^n - 1} \quad (7)$$

Where (n) is the lifetime of the Regenerative ORC system, and (i) is the interest rate. Table 3 provides the specification of the economic parameter. The "Levelised Energy Cost (LEC)" is obtained as follows:

$$LEC = \frac{C_{RF}.C_{CC,2022} + C_{OM}}{T_{OM}.W_{net}} \quad (8)$$

Where T_{om} is the number of hours of operation in a year, and C_{OM} is the cost of operation and maintenance, which is calculated as 1.5% of $C_{CC,2022}$.

The definition of the "Static investment payback period (SIPP)" is as follows:

$$SIPP = \frac{C_{cc,2022} + C_{OM}}{I_r} \quad (9)$$

Where I_r revenue per hour from reclaiming waste heat for energy production is expressed as:

$$I_r = \eta_{System}.\dot{m}(h_{Wasteheat.in} - h_{Wasteheat.out}).C_{electricity} \quad (10)$$

The term "$C_{electricity}$" in the equation above stands for the price of electricity, which is assumed to be 0.1512 USD/kWh, and refers to the industrial pricing that the U.S. Energy Information Administration published for the year 2022 (U.S. Energy Information Administration 2022).

Table 2. The coefficient of capital cost estimation model (R. Turton, R.C. Bailie 2013).

Components	Y	K_1	K_2	K_3	F_{BM}	Units, Capacity
Condenser, Evaporator, and Recuperator (Fixed Tube)	$A_{eva}(m)^2$, Heat Transfer area	4.3247	-0.3030	0.1634	2.9	Area, m^2 (100-4000)
Turbine (Radial)	$W_{Turbine}(kW)$, Power capacity	2.476	1.4965	-0.1618	3.5	kW (100-1500)
Pump (Centrifugal)	$W_{pump}(kW)$, Power capacity	3.3892	0.0536	0.1538	2.8	kW (1-300)

2.5 Optimisation outline

The optimisation study using the NSGA II technique was started with four parameters- HT pressure ORC, LT pressure ORC, Massflow of ORC working fluids, and waste heat temperature. The maximum overall efficiency has always been observed at the optimal values (maximum and minimum of the given range). Throughout the optimisation simulation, it has been ensured that the high-temperature pressure in the turbine inlet is consistently higher than the low-temperature pressure at the turbine outlet. The NSGA-II algorithm is based on Pareto dominance, which evaluates the quality of candidate solutions. NSGA-II generates a collection of Pareto-optimal solutions that reflect the balance between the optimised objectives. This study presents a comparative analysis between the outcomes of NSGA II with other Pareto-optimal solutions methods, namely TOPSIS, GRA, SAW, and MABAC (Wang and Rangaiah 2017) (Wang et al. 2020) (Wang et al. 2021). Table 4 provides the relevant NSGA-II parameters. Table 3 provides the relevant NSGA-II parameters.

Table 3: Specification of the parameters used in economic analysis.

Parameters	Value	Ref.
i	14 %	(Mosaffa et al. 2017)
n	15 Years	(Mosaffa et al. 2017)
Operation and Maintenance Cost	1.5%	(Mosaffa et al. 2017)
Operation hours	7300 h	(Mosaffa et al. 2017)

2.2.1 Objective Function

The regenerative ORC system's multi-objective optimisation (MOO) design problem is formulated. The primary objective of MOO research is to maximise energy efficiency (percentage) while decreasing Levelized energy costs (USD/kWh)$^{-1}$. The MOO optimisation problem is constructed such that the high side pressure of the turbine is always more significant than the low side pressure. In addition to the design space, the working fluid's massflow rate and the waste heat's temperature are included as optimisation parameters. The MOO issue is described as follows:

$$Max = \eta_{ex}, f\left(W_T, P_{in}, P_{out}, m_{ORC,}\right) \quad (11)$$

$$Min = LEC, f\left(W_T, P_{in}, P_{out}, m_{ORC,}\right) \quad (12)$$

Subject to:

$$(P_{in} > P_{out} \geq P_0)$$

737

There are two types of operational parameters; fixed parameters are constant throughout the study, while variable parameters can be modified within the set limitations to enhance the cycle performance. Referring to the WHR cycle in Figure 1, The general form of the objective function is expressed as follows: where waste heat temperature Input and the output pressure of turbine and massflow of the working fluid.

Table 4: NSGA II parameters used in the present study.

Parameter	Values
Population size	50
Number of generations	70
No. of objectives	2
No. of variables	4
Mutation type	Gaussian
Crossover type	Intermediate
Scale	0.1
Shrink	0.5

2.6 Modelling assumptions

The modelling assumption parameters are displayed in Table 5. Fixed and variable parameters are used in this work, and values for fixed parameters are carefully selected from the literature.

3 RESULTS AND DISCUSSION

According to the waste heat temperature shown in Table 1, the working fluids for this work have been chosen. Also, the waste heat temperature range is being optimised based on the waste heat range of each working fluid. The maximum temperature range for waste heat is 225 °C to 300 °C. This range includes benzene, Toluene, and Heptane. 200 °C to 275 °C is the medium waste heat temperature range. MM,

Cyclopentane, Pentane, and Hexane have been identified in this range. Butane (125 °C to 200 °C) has the lowest temperature range. After that, all the recommended working fluids were tested in the regenerative ORC system's subcritical range of turbine inlet and outlet pressure, where the inlet pressure is always greater than the outlet pressure. The working fluids massflow rate, which varies from 1 to 30 kg/s for each fluid, is another significant variable component. NSGA II is used to identify the most effective working fluid in various waste heat ranges based on these optimisation functions.
The Pareto frontiers for the outcomes of levelized energy costs and energy efficiency optimisation across working fluids using NSGA-II are displayed in Figure 2. For each working fluid, the best compromise solution was found by balancing the maximum energy efficiency and the minimum levelized energy cost. The Pareto frontier consisted of 3500 optimal ideal solutions for all working fluids. The economic weight is not necessarily equal to the thermodynamic weight due to practical requirements and choices. However, for this research, all working fluids have the same weight (0.5) for both objective functions.

Table 5: The accepted nominal parameters for the designed Regenerative ORC.

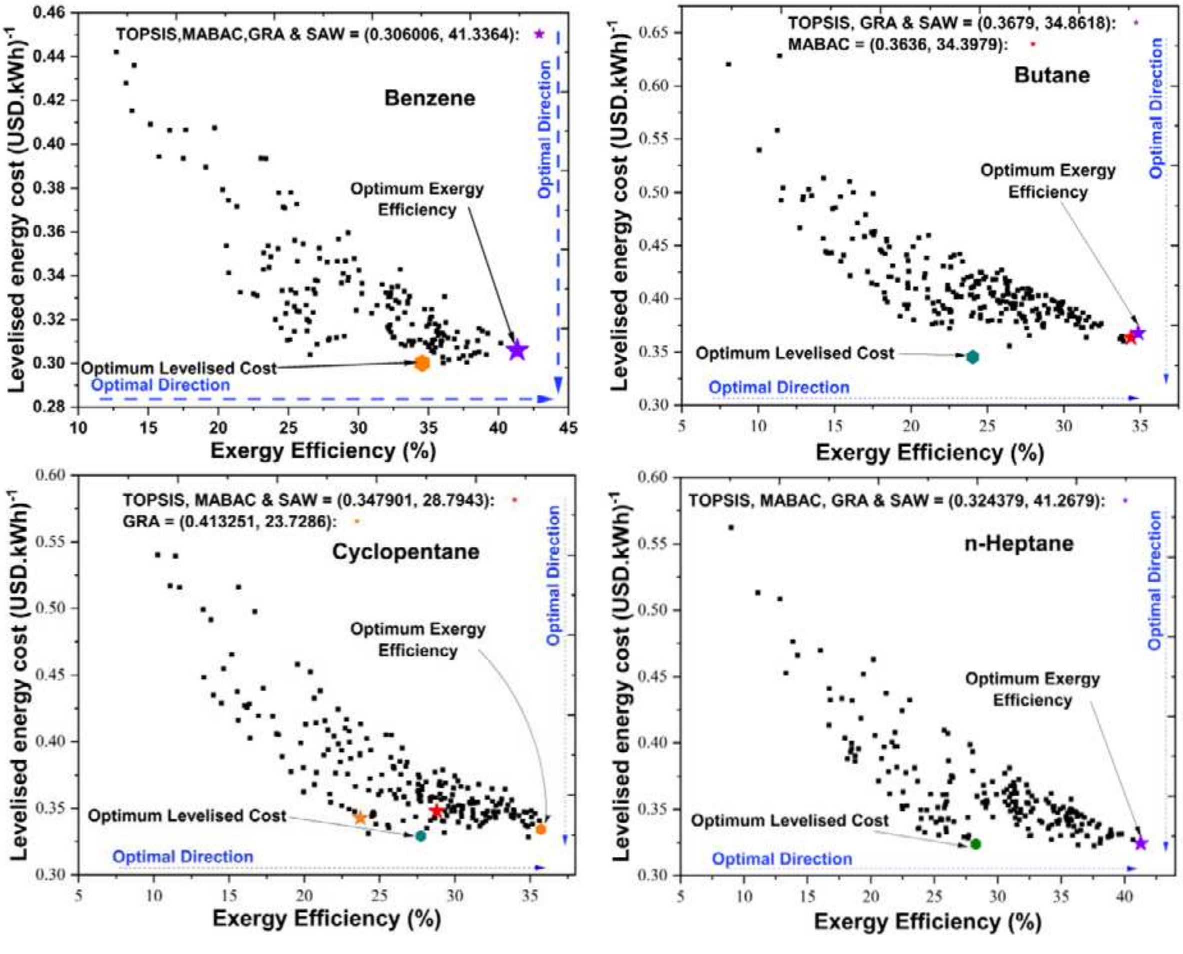
Operating parameter	Value/range	Unit
Fixed Design Parameter		
Exhaust gas composition	Air	-
Exhaust gas pressure	1	bar
Exhaust gas mass flow rate (Köse et al. 2020)	12	kg/s
Isentropic efficiency of the pump (DiPippo 2015)	85	%
Isentropic efficiency of the turbine (Gopal and Seshadri 2022)	85	%
Isentropic efficiency of the compressor (Hoque and Kumar 2021)	75	%
Pump input temperature	40	°C
Ambient temperature	35	°C
Pipes pressure drops (El Samad et al. 2020)	0	bar
Pinch temperature of condenser, recuperators, and heater (El Samad et al. 2020)	5	°C
Pressure drops in the heat exchanger, recuperators, and condenser (Wang et al. 2014)	1.5	bar
Variable Design Parameter		
Exhaust gas temperature (W_T)	125-300	°C
ORC Turbine inlet pressure (P_{in})	1- 40	bar
ORC Turbine outlet pressure (P_{out})	1- 40	bar
ORC Turbine inlet mass flow rate (m_{ORC})	1-30	kg/s

As mentioned, the waste heat's temperature determines which working fluid to use. So, using the multiple criteria decision-making (MCDM) technique with TOPSIS, GRA, and SAW, the best compromise solutions for Butane have been found as ordered pairs of values (exergy efficiency in percentage, LEC) of (34.86, 0.36) and the MABAC (34.39, 0.36) for the lowest temperature range. According to the results, TOPSIS, GRA, and SAW all provided the same value for Butane; therefore, this value is the strongest value accepted for the best compromise solutions.
Cyclopentane, Pentane, MM, and Hexane are chosen for the medium temperature range (200 - 275 °C) investigation. The best compromise solutions for MM, Pentane, and Hexane have been identified as ordered pairs of values (exergy efficiency in %, LEC) of (29.75, 0.43), (34.39, 0.36), and (35.28, 0.34), respectively, using the multiple criteria decision-making (MCDM) technique with TOPSIS, MABAC,

GRA, and SAW. The ordered pairs of values (exergy efficiency in %, LEC) for TOPSIS, MABAC, and SAW that represent the optimum compromise option for Cyclopentane is (28.79, 0.34) and the GRA result is (23.72, 0.41). Considering the findings, the value offered by TOPSIS, GRA, MABAC, and SAW for MM, Pentane, and Hexane is the most substantial value acknowledged for optimum compromise options. TOPSIS, MABAC, and SAW offered the best compromise solutions for Cyclopentane.

A higher waste heat temperature range (225–300 °C) has been used for this study. Heptane, Toluene, and Benzene are the hydrocarbons selected for this temperature range. Using the multiple criteria decision-making (MCDM) technique with TOPSIS, MABAC, GRA, and SAW, the best compromise solutions for Heptane, Toluene, and Benzene have been identified as ordered pairs of values (exergy efficiency in%, LEC) of (41.26, 0.32), (42.75, 0.29), and (41.33, 0.30), respectively. The value provided by TOPSIS, GRA, MABAC, and SAW for Heptane, Toluene, and benzene is the most critical value acknowledged for the best compromise options, according to the findings. Toluene has emerged as the best solution for higher temperatures regarding the best working fluid. Hexane is the best working fluid for medium temperature ranges, and Butane has the best solution for applications with the lowest waste heat temperature range.

Table 6 displays the ranking obtained from the SIPP calculation and the optimal values of the objective functions. The working fluid Butane requires 11650.98 hours of operation and maintenance and covers the capital cost of the Regenerative ORC based on the lowest range of waste heat temperature. Pentane has the shortest recovery time for waste heat temperatures in the middle range, 10837.29 hours. Other medium-range working fluids underperform, including hexane, mm, and cyclohexane. In the higher temperature range, Heptane has the shortest recovery time, 11578.54 hours, to recover the value of operation and maintenance and cover the capital cost, while Benzene and Toluene perform poorly because their SIPP values exceed 19987.7 hours.



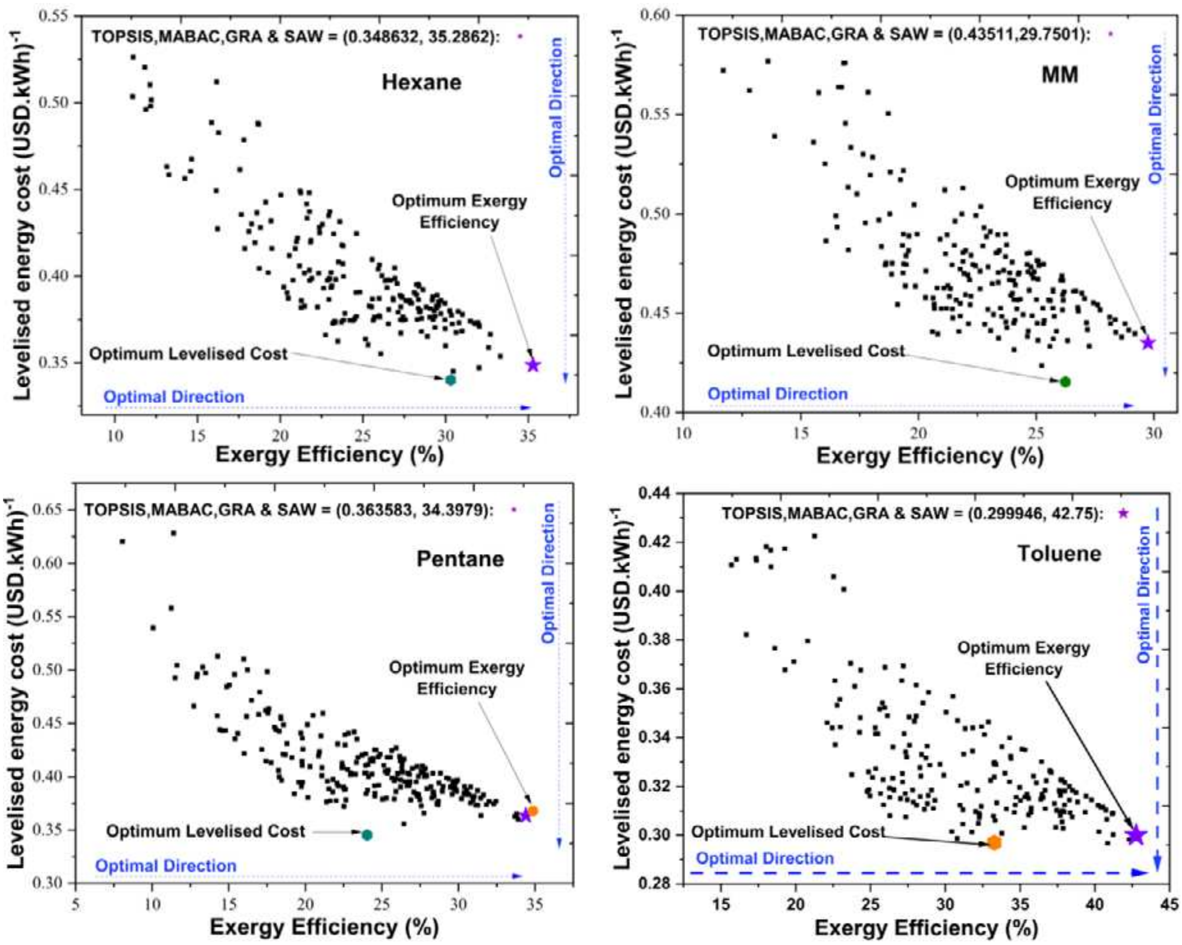


Figure 2: Optimal compromise solution on the Pareto frontiers of eight candidates: Benzene, Butane, Cyclopentane, Heptane, Hexane, MM, and Toluene.

Table 6: Optimum values of the objective function and SIPP ranking.

Working Fluid	Waste heat temperature range (T_w)	Waste heat temperature (°C)	Massflow rate (kg/s)	Pressure Turbine inlet (bar)	Pressure Turbine outlet (bar)	SIPP (hrs.)
Benzene	250-300	290.0	0.500	42.66	1.25	20879
Butane	125-200	226.0	0.763	39.66	3.76	11650
Cyclopentane	200-275	298.9	0.644	20.21	1.75	22184
Heptane	225-300	244.0	0.538	22.09	1.12	11578
Hexane	200-275	259.0	0.528	13.35	1.37	11837
HexMDiSiloxn (MM)	200-275	267.5	0.522	16.35	1.61	18250
Pentane	200-275	232.5	0.519	11.70	1.45	10837
Toluene	275-300	298.9	0.514	18.11	1.83	19987

4 CONCLUSIONS

This article examined a regenerative ORC cycle based on the distinctive properties of eight different working fluids. The Pareto frontier for all working fluids contained 3500 optimal ideal solutions using MOO. The best compromise options were found using the MCDM method using TOPSIS, GRA, and SAW. Waste heat temperature ranges are optimised for each working fluid. The maximum waste heat range is 225–300°C. Benzene, Toluene, and Heptane are included in this range. Medium waste heat temperatures are 200–275 °C. This range includes MM, Cyclopentane, Pentane, and Hexane. Butane (125–200°C) has the lowest temperature range. After completing the optimisation process, Regenerative ORC with Toluene generated the highest exergy efficiency and LEC, 57.5% and 0.31, respectively. Using the multiple criteria decision-making (MCDM) technique with TOPSIS, MABAC, GRA, and SAW, the best compromise solutions for medium temperature range hexane have been identified as ordered pairs of values (exergy efficiency in%, LEC) of 35.28 and 0.34, respectively. Butane was found as values of (exergy efficiency in percentage, LEC) for the lowest temperature range for TOPSIS, GRA, and SAW (34.86, 0.36) and MABAC (34.39, 0.36). In the SIPP index, Pentane has the shortest recovery time for waste heat temperatures in the middle range, 10837.29 hours, compared to all other working fluids.

NOMENCLATURE

$\dot{m}$	mass flow rate	kg/s	s	entropy	kJ/kg K
h	enthalpy	kJ/kg	η	efficiency	
W	work	kW	P	pressure	bar
T	Waste heat	°C			

Subscript

0	reference/ambient	out	output
in	Input		

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The present piece of work is dedicated to the memory of Sidharth Sankar Parhi, who unfortunately passed away during the Covid pandemic. During the process of conception, he played an active role as a member of this work.

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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