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Abstract

The Organic Rankine Cycle (ORC) offers a promising solution for converting low-grade heat into The Organic Rankine Cycle (ORC) is an effective and innovative approach for converting low-grade heat into electricity by utilizing organic fluids with suitable thermodynamic properties. This study examines how different working fluids affect the efficiency of the ORC across various configurations. Through a combination of experimental testing and simulation, the research identifies five fluids (Cyclopentane, Dichloromethane, n-Pentane, R113, and R141b) as top performers under different operating conditions. The findings clearly show that the choice of working fluid plays a vital role in improving the overall performance of the ORC system. Furthermore, this study highlights the importance of selecting the appropriate fluid to maximize energy recovery and enhance system reliability. The flexibility of ORC technology is emphasized, demonstrating its potential as an efficient and adaptable solution for reducing energy waste and optimizing resource utilization in industrial applications. Ultimately, the results underline the significant benefits of ORC in increasing energy efficiency and promoting sustainable energy practices, paving the way for broader adoption of clean and environmentally friendly power generation technologies.

*Keywords:* Rankine Cycle, GAMS, Fluid selection;

1. **Introduction**

Growing concerns over energy security and environmental sustainability underscore the need for efficient utilization of waste-heat streams in industrial processes. [1]A significant portion of the input energy in production systems is dissipated to the environment as unused thermal energy, which not only leads to substantial energy losses but also contributes to greenhouse-gas emissions. Among emerging waste-heat recovery technologies, the Organic Rankine Cycle (ORC) has attracted considerable attention due to its ability to operate with low- to medium-temperature heat sources and its flexibility in employing organic working fluids with low boiling points. These advantages enable ORCs to be deployed across a wide range of applications, including geothermal, solar, biomass, and industrial waste-heat recovery.

In recent years, research in this field has evolved from purely thermodynamic analyses toward multi-objective optimization and hybrid approaches. For instance, Palma-Flores et al. (2015; 2016) proposed pioneering frameworks for assessing ORC working fluids by integrating thermodynamic and economic perspectives, highlighting the importance of coupling technical and cost evaluations[2, 3]. More recent studies emphasize performance enhancement and environmental benefits: Oyekale et al. (2020) demonstrated that employing siloxane mixtures in solar–biomass ORC systems can significantly improve exergy efficiency and reduce CO₂ emissions[4]. Similarly, Wang et al. (2024) developed a multi-objective optimization framework that simultaneously accounts for capital cost, thermal efficiency, and environmental performance, thereby providing a roadmap for sustainable ORC design[5]. Furthermore, the recent review by Damarseckin (2024) suggests that the future of ORCs lies in their integration with smart-energy networks and renewable-based hybrid systems[6].

Despite these advancements, several critical research gaps remain. First, most investigations have focused on conceptual design and thermodynamic modeling, whereas industrial-scale operational evaluation has been underexplored. Second, many studies consider only a single configuration, limiting systematic comparisons across different ORC layouts. Third, there is a lack of integration between equation-based mathematical optimization and process-simulation validation, which is essential to bridge the gap between theory and practical deployment.

Motivated by these gaps, the present study addresses the design and optimization of two ORC configurations—a basic cycle and a recuperated cycle—by employing GAMS for mathematical optimization and Aspen HYSYS for process validation. This integrated approach not only enhances understanding of the interaction between working-fluid selection, operating conditions, and cycle efficiency, but also provides a practical roadmap for the industrial implementation of sustainable ORC systems.

Figure 1. Rankine cycle for Config. A [4]

In the following, the thermodynamic modeling of the ORC (Organic Rankine Cycle) is examined. To model this cycle using various assumptions, three different approaches for the thermodynamic simulation of the cycle showen in Figure 1.

1. **Problem statement**

Our goal is to convert low- to medium-grade waste heat into electricity using an organic Rankine cycle (ORC) under realistic industrial constraints and formulate the optimization in an equation-oriented (EO) manner suitable for exact solutions.

A single hot-water stream is the heat source. The sink is an air-cooled condenser. Two ORC configurations are analyzed under identical boundary conditions:

• Configuration A (simple cycle): evaporator → turbine → condenser → pump

• Configuration B (recuperated cycle): the simple cycle augmented with an internal heat exchanger (recuperator) that preheats the working fluid using turbine exhaust

We consider a set of at least five pure working fluids drawn from the recommended list and literature. Thermophysical constants (Tc, Pc, omega, MW) are treated as known for each candidate. Heat‑capacity treatment follows the model: Cp(T) polynomials if available, otherwise a constant cp\_avg. The optimal fluid is selected within the optimization (or via a screen–then–solve protocol) while ensuring that only one pure fluid is active in each run.

Thermophysical modeling: Property calculations use the Peng–Robinson (PR) equation of state. A stable cubic‑root selection consistent with liquid/vapor phases (Kamath‑compatible handling) provides compressibility Z and departure functions. Ideal‑gas enthalpy uses Cp(T) polynomials if present, otherwise a constant \*C**pa**v\*\*g\*.

It is assumed that the outlet flow from the evaporator is the lowest possible value considering the outlet water inlet outside 165°C and since stream 1 is the inlet to the turbine, we assume all the flow is vapor. Stream 2 is assumed to be the turbine outlet once and also the water pressure of stream 3 is assumed to be completely liquid with respect to the material point so that the inlet to the pump is completely liquid. The pressures of streams (1,4) and (2,3) are equal considering that we have pressure drops in the heat exchangers.

For fair comparisons against flowsheet simulations, matched boundary conditions (source/sink), identical fluid identity and property package, and consistent unit systems are required. Differences in fluid choice, bounds, or property methods can materially change *W*\*t**u**r**b *and* Wn**e\*\*t\*.

In this approach, five components -Cyclopentane, Dichloromethane, n-Pentane, R113, and R141b- are selected.

1. **Problem formulation**

The given specifications are listed in Table 1.

Table 1. Source/sink and equipment data (nominal)

Item

Value

Units

Hot-water pressure

10

bara

Hot-water inlet temperature

443.15

K

Hot-water outlet temperature

343.15

K

Hot-water mass flow

100

kg/s

Cooling air inlet temperature

298.15

K (25 °C)

Water heat capacity

4.675

kJ/(kg\*K)

Condenser approach

5

K

Evaporator pinch

5

K

Pump isentropic efficiency

0.75

-

Turbine isentropic efficiency

0.80

-

Generator efficiency

0.95

-

To determine the enthalpy of each stream, Equation 1 is used. The actual enthalpy of each stream includes three to four parameters: the ideal gas enthalpy, the residual enthalpy indicating the deviation from the ideal state, the formation enthalpy which is a constant value for the substance, and if the substance is in the liquid phase, the enthalpy of vaporization should be added to the actual enthalpy.

*Hr****e****a****l = Hi****g* + *Hr****e****s* + *Hf****o****r****m + Hv****a****p      e****q*.1

If the stream is two-phase, Equation 2 must be used, which calculates the enthalpy for saturated vapor and liquid, and then the vapor fraction of the stream is inserted into the equation to obtain the actual enthalpy.

*H* = *v****a****p*. *f****r****a****c \* HS****a****t.v****a****p + (1 − v****a****p. f****r****a****c*) \* *HS****a****t*.*l****i****q*  \*e\*\*q\*.2

To calculate the ideal gas enthalpy of a stream, Equation 3 is used. Coefficients a to f are read from the Aspen HYSYS software, and by inputting the temperature in Kelvin into Equation 3, the ideal gas enthalpy (Kj / Kg) is obtained.

*Hi****g = a + b****T* + *c****T2 + d****T*3 + *e****T4 + f****T*5     \*e\*\*q\*.3

To calculate the second parameter in Equation 1, the residual enthalpy, existing EOS[1] are used. Considering the problem’s requirements, the PR[2] equation of state is chosen. Using the relations provided in [7], presented as Equations 4 to 12, the desired parameter is calculated. To solve the cubic equation in Equation 5, the Kamath method is used.

$H^{Res} = RT\left( Z - 1 - \frac{A}{B\sqrt{8}}\left( 1 + \frac{m\sqrt{T\\_{r}}}{\sqrt{\alpha}} \right)\ln\left\lbrack \frac{Z + \left( 1 + \sqrt{2} \right)B}{Z + \left( 1 - \sqrt{2} \right)B} \right\rbrack \right)\\\\\\\\$eq.4

*Z*3 − (1 − *B*)*Z*2 + (*A* − 2*B* − 3*B*2)*Z* − (\*A\*\*B*−*B*2 −*B\*3) eq.5

eq.6

*α*= [1 + *m*(1 − *Tr*0.5)]2 eq.7

*m* = 0.375 + 1.54*ω* − 0.27*ω*2 eq.8

$a = 0.457235\\\frac{R^{2}T\\_{C}^{2}}{P\\_{C}}\\*\\\alpha$ eq.9

$b = 0.077796\\\frac{RT\\_{c}}{P\\_{C}}$ eq.10

eq.11

eq.12

Assuming the purity of each stream, by substituting either the temperature or pressure of a stream, other parameters of that stream, such as the fugacity coefficient (Equations 13 & 14) or the compressibility factor, can be calculated.

*f****o****r* *p****u****r****e s****y****s****t****e****m*→ *φv* = *φl* eq.13

eq.14

To find the molar flow rate of the pure component in the cycle, Equation 15 is used, which determines the molar flow rate of the component by balancing the energy in the cycle’s evaporator.

*ṅ*(*H*1 − *H*4)= *ṁwCp*, *w*(Δ*T* − 5)       \*e\*\*q\*.15

Subsequently, the thermodynamic parameters of the mentioned cycle are calculated, and the pump’s required work is determined using Equation 16 & 17. Finally, the turbine’s generated work is calculated using Equation 18.

$$\mathrm{\Delta}H\\_{pump} = \\\frac{\left( P\\_{4} - P\\_{3} \right)\\*\dot{n}\\*MW}{density}\\\\\\\\\\\\\\\\eq.16$$

$$W\\_{pump} = \\\frac{\mathrm{\Delta}H\\_{pump}}{\eta\\_{pump}}\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\eq.17$$

*Wt****u****r****b****i****n****e*= *ṅ*(*H*1 − *H*2)               \*e\*\*q\*.18

Given that the fluid at the turbine inlet must be steam and the heating fluid is water, the boiling point of the selected fluid must be lower than the boiling point of water (100 degrees Celsius).

Also, the fluid at the inlet of the flow pump 3 is completely liquid. And given the cooling air temperature of 25 degrees, the best case scenario is that the outlet from the cooler can be 30 degrees Celsius, so fluids whose boiling points are higher than 30 degrees Celsius should be selected.

Given these constraints, 16 fluids (table 2) were selected, of which these three fluids (Actone, Ethanol, FC72) were also removed due to their inappropriateness for the Ping-Robinson equations (due to the warning of the Hysys software), and also the fluid (R124) can liquefy at temperatures much lower than 30 degrees, and its boiling point is probably incorrectly stated as 36.1 in the Excel file.

Table 2. Selected fluids.

Name

Tb@ 1 bar

1

2,2-dimethylbutane

49.73101

2

4-methyl-2-pentene

58.58

3

Acetone

56.07

4

Benzene

80.06

5

Cyclopentane

49.24801

6

Dichloromethane

39.85

7

Ethanol

78.15

8

FC72

55.9

9

Isohexane

60.11

10

Methanol

64.54

11

n-heptane

97.9

12

n-hexane

69.18

13

n-pentane

35.78

14

R113

47.57

15

R124

36.1

16

R141b

31.99999

1. **Results and discution**

نتایج قسمت A

| Spec | Hysys | GAMS | Error% | توضیح |
| --- | --- | --- | --- | --- |
| Wt | 8699.537 | 44853.5 | -415.585 | Heat Flow [kJ/s] |
| Wp | 242.70688 | 242.803 | -0.0396 | Heat Flow [kJ/s] |
| Molar Flow | 1.3898043 | 1.39 | -0.01408 | [kgmole/s] |
| H1 | -90102.27 | -90025.2 | 0.085523 | Molar Enthalpy [kJ/kmole] |
| H2 | -96361.81 | -122292 | -26.9095 | Molar Enthalpy [kJ/kmole] |
| H4 | -122262.9 | -121975 | 0.235481 | Molar Enthalpy [kJ/kmole] |
| P1 | 20.959427 | 20.985 | -0.12201 | Pressure [bar] |
| T2 | 312.40593 | 312.409 | -0.00098 | Temperature [K] |
| T4 | 313.24878 | 313.151 | 0.031215 | Temperature [K] |

Here is the data from the spreadsheet in the image:

| Hysys | Name | Wp | Wt | Wnet(Kj/s) |
| --- | --- | --- | --- | --- |
| 1 | 2,2-dimethylbutane | 258.134799 | 6839.564 | 5213.5163 |
| 2 | 4-methyl-2-pentene | 219.5780021 | 6365.124 | 4872.8213 |
| 3 | Acetone | 56.07 |  |  |
| 4 | Benzene | 92.17404287 | 5588.065 | 4378.2778 |
| 5 | Cyclopentane | 221.3920083 | 7617.756 | 5872.813 |
| 6 | Dichloromethane | 242.7068797 | 8699.537 | 6716.9227 |
| 7 | Ethanol | 78.47 |  |  |
| 8 | FC72 | 65.9 |  |  |
| 9 | Isohexane | 205.8012394 | 6114.503 | 4685.8008 |
| 10 | Methanol | 108.9162242 | 6929.143 | 5434.3979 |
| 11 | n-heptane | 71.80336678 | 3557.273 | 2774.0151 |
| 12 | n-hexane | 166.2908911 | 5674.165 | 4373.0408 |
| 13 | n-pentane | 344.476657 | 7579.137 | 5718.8307 |
| 14 | R113 | 278.818838 | 7197.7 | 5479.2284 |
| 15 | R124 | 36.6 |  |  |
| 16 | R141b | 362.5213291 | 8510.272 | 6445.6959 |

نتایج: با توجه به جواب مدلسازی، سیال انتخاب‌شده همان سیال HYSYS است؛ خطا در اکثر متغیرها مناسب است و فقط کار توربین و آنتالپی جریان ۲ نیاز به بهبود دارند.

نتیجه: با توجه به ۵ سیال انتخاب‌شده، سیالات با جرم مولکولی بزرگ‌تر W\_net بزرگ‌تری ایجاد کرده‌اند؛ مطابق ادبیات (1,2).

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3. **Conclutions**

References [Appendix – Added Results (as requested)]

نتایج قسمت A

| Spec | Hysys | GAMS | Error% | توضیح |
| --- | --- | --- | --- | --- |
| Wt | 8699.537 | 44853.5 | -415.585 | Heat Flow [kJ/s] |
| Wp | 242.70688 | 242.803 | -0.0396 | Heat Flow [kJ/s] |
| Molar Flow | 1.3898043 | 1.39 | -0.01408 | [kgmole/s] |
| H1 | -90102.27 | -90025.2 | 0.085523 | Molar Enthalpy [kJ/kmole] |
| H2 | -96361.81 | -122292 | -26.9095 | Molar Enthalpy [kJ/kmole] |
| H4 | -122262.9 | -121975 | 0.235481 | Molar Enthalpy [kJ/kmole] |
| P1 | 20.959427 | 20.985 | -0.12201 | Pressure [bar] |
| T2 | 312.40593 | 312.409 | -0.00098 | Temperature [K] |
| T4 | 313.24878 | 313.151 | 0.031215 | Temperature [K] |

Here is the data from the spreadsheet in the image (Part A candidates):

| Hysys | Name | Wp | Wt | Wnet(Kj/s) |
| --- | --- | --- | --- | --- |
| 1 | 2,2-dimethylbutane | 258.134799 | 6839.564 | 5213.5163 |
| 2 | 4-methyl-2-pentene | 219.5780021 | 6365.124 | 4872.8213 |
| 3 | Acetone | 56.07 |  |  |
| 4 | Benzene | 92.17404287 | 5588.065 | 4378.2778 |
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| 11 | n-heptane | 71.80336678 | 3557.273 | 2774.0151 |
| 12 | n-hexane | 166.2908911 | 5674.165 | 4373.0408 |
| 13 | n-pentane | 344.476657 | 7579.137 | 5718.8307 |
| 14 | R113 | 278.818838 | 7197.7 | 5479.2284 |
| 15 | R124 | 36.6 |  |  |
| 16 | R141b | 362.5213291 | 8510.272 | 6445.6959 |

نتایج: سیال انتخاب شده همان سیال HYSYS است؛ اغلب خطاها کوچک‌اند و فقط کار توربین و آنتالپی جریان ۲ انحراف دارند.

نتیجه: از بین ۵ سیال انتخابی، سیالات با جرم مولکولی بزرگ‌تر W\_net بیشتری ایجاد کرده‌اند؛ مطابق ادبیات (1,2) درباره معیار دمای بحرانی.

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[1] Equations of State

[2] Peng Robinson