

Supplementary Material

S1. Numerical implementation and thermophysical properties

The ORC model is implemented in MATLAB (R2023a, MathWorks Inc.) to solve the component-wise mass and energy balances and to evaluate the cycle state points under prescribed boundary conditions. Thermophysical properties of the candidate working fluids are obtained from REFPROP (v10.0) to ensure a single, internally consistent property source across the investigated temperature and pressure ranges[3]. This consistent property evaluation is important for fair working-fluid screening and for the subsequent parametric and multi-objective optimization, where property inconsistencies may otherwise bias comparisons among fluids.

The multi-objective optimization is carried out using the NSGA-II algorithm via the *pymoo* implementation, where the decision variables, objectives, and feasibility constraints follow the definitions in the main text. The numerical settings (solver strategy, convergence criteria, and software/package versions) are reported here to support reproducibility while keeping the main manuscript focused on the modelling assumptions, constraints, and decision-oriented outputs.

For completeness, we note that several geothermal/ORC software tools are available for performance and techno-economic assessment (e.g., GEOPHIRES-X, GeoT*SOL, ORCmKit, and ORCSimulator). These tools are valuable for their intended use cases; however, they are not designed to natively support the specific end-to-end coupling required in this work, namely multi-fluid screening under identical boundary conditions, consistent thermo-/exergoeconomic evaluation, explicit feasibility constraints embedded in the search (e.g., pinch-point limits and superheat/subcooling requirements), and automated multi-objective optimization (NSGA-II) over a large number of candidate solutions. Implementing the present workflow therefore requires a transparent, scriptable numerical back-end in which the governing models, constraints, and optimization loop can be fully specified and reproduced.

S2. Detailed models and correlations

S2.1. First law model

The system simulation and calculation of state point parameters are based on the given heat source temperature T_9 and mass flow rate $\dot{m}_9$. For the evaporator and condenser analysis, the pinch point temperature differences $\Delta T_{pp,ev}$ and $\Delta T_{pp,cn}$ are crucial. These differences affect the heat exchangers' performance and the temperatures at the reinjection point T_{10} and the cooling water exit T_6 . Additionally, for certain working fluids, the turbine outlet (Point 4) may be in a liquid state, posing a risk to turbine operation. Therefore, superheating at the turbine inlet is considered to mitigate this risk. To prevent cavitation at the pump inlet, subcooling is also considered in the simulation[4].

In the analysis based on the first law of thermodynamics, the equations describing the pumps can be summarized as follows:

$$\eta_{orc,p} = \frac{h_{2s} - h_1}{h_2 - h_1} \quad (S1)$$

$$\dot{W}_{orc,p} = \dot{m}_1 \cdot (h_2 - h_1) \quad (S2)$$

$$\dot{W}_{hp} = \frac{\dot{m}_9 \cdot dP_{w,ev}}{\rho_w \eta_{hp}} \quad (S3)$$

$$\dot{W}_{cp} = \frac{\dot{m}_5 \cdot dP_{w,cn}}{\rho_w \eta_{cp}} \quad (S4)$$

The governing equations for the evaporator and condenser are:

$$\dot{Q}_{ev} = \dot{m}_1 \cdot (h_3 - h_2) = \dot{m}_9 \cdot (h_9 - h_{10}) \quad (S5)$$

$$\dot{Q}_{cn} = \dot{m}_1 \cdot (h_4 - h_1) = \dot{m}_5 \cdot (h_6 - h_5) \quad (S6)$$

The governing equations for the turbine expander are:

$$\eta_t = \frac{h_3 - h_4}{h_3 - h_{4s}} \quad (S7)$$

$$\dot{W}_t = \dot{m}_1 \cdot (h_3 - h_4) \quad (S8)$$

Based on the thermal energy input to the ORC system, the first law efficiency of the system can be expressed as:

$$\eta_I = \frac{\dot{W}_{net}}{\dot{Q}_{ev}} = \frac{\dot{W}_{elec} - \dot{W}_{orc,p} - \dot{W}_{hp} - \dot{W}_{cp}}{\dot{Q}_{ev}} \quad (S9)$$

S2.2. Second law model

Compared to the first law analysis, which only considers energy conversion efficiency, the second law analysis, which considers the efficiency of available energy utilization, usually receives more attention for low-temperature heat source utilization systems like ORC[5, 6]. Complete exergy calculation includes physical exergy, chemical exergy, kinetic exergy, and potential exergy[7]. Given that there are no chemical changes in the ORC system and changes in kinetic and potential energy are negligible, the second law analysis only considers the physical exergy of each stream:

$$\dot{E}_i = \dot{E}_{i,ph} = \dot{m}[(h_i - h_0) - T_0(s_i - s_0)] \quad (S10)$$

The exergy balance for an open thermodynamic system can be expressed as:

$$\sum \dot{E}_{input} - \sum \dot{E}_{output} = \dot{I} \quad (S11)$$

The exergy loss for each component is given by the following equation:

$$\dot{I}_{orc,p} = \dot{W}_{orc,p} + \dot{E}_1 - \dot{E}_2 \quad (S12)$$

$$\dot{I}_{ev} = \dot{E}_9 + \dot{E}_2 - \dot{E}_{10} - \dot{E}_3 \quad (S13)$$

$$\dot{I}_{cn} = \dot{E}_4 - \dot{E}_1 \quad (S14)$$

$$\dot{I}_t = \dot{E}_3 - \dot{W}_t - \dot{E}_4 \quad (S15)$$

S2.3. Exergoeconomic model

In addition to thermodynamic performance, the economic performance of ORC systems is crucial. Common indicators such as Specific Investment Cost (SIC), Payback Period (PBP), and Levelized Cost of Electricity (LCOE) are often used[1]. However, these indicators may not accurately capture the unique characteristics of ORC systems, which often exhibit lower efficiencies. Optimizing ORC systems using these indicators can make it challenging to define their economic benefits relative to other thermodynamic cycles.

Introducing Exergoeconomic analysis is beneficial as it combines exergy and economic analysis to evaluate each component's importance within the system. This comprehensive approach enhances the understanding of both thermodynamic and economic aspects of ORC system optimization. The methodology used in this study is based on Specific Exergy Costing (SPECO), which defines the fuel and product costs for all components based on their exergy streams and applies commercial management principles to calculate system costs[8]. Conducting an exergoeconomic analysis requires applying cost balance and auxiliary equations to each component. If there are N exergy

streams exiting a component, there will be N unknowns and one cost balance equation, necessitating $N - 1$ auxiliary equations, established using the Pand F principles of the SPECO method.

The cost balance equation can be described as:

$$\sum \dot{C}_{o,k} = \sum \dot{C}_{i,k} + \dot{Z}_k \quad (S16)$$

Where $\dot{C}$ represents the cost rate associated with the exergy streams entering and exiting the component under consideration. It can be further broken down into cost rates related to thermal energy, electrical energy, and the exergy stream itself:

$$\dot{C}_{heat} = c_{heat} \dot{E}_{heat} \quad (S17)$$

$$\dot{C}_{work} = c_{work} \dot{W} \quad (S18)$$

$$\dot{C}_i = c_i \dot{E}_i \quad (S19)$$

The total cost rate $\dot{Z}_k$ includes capital investment and operating and maintenance expenses for the k -th component[9,10]:

$$\dot{Z}_k = \dot{Z}_k^{CI} + \dot{Z}_k^{OM} \quad (S20)$$

In this study, the capital investment for the components is considered as the purchase cost (PEC). To evaluate the cost-effectiveness of different financing schemes over the lifespan of geothermal power plants, the capital investment is annualized:

$$\dot{Z}_k^{CI} = \left(\frac{CRF}{X} \right) \times (PEC) \quad (S21)$$

Where CRF is the Capital Recovery Factor, X is the annual operating hours of the ORC geothermal power plant.

The CRF is calculated using the interest rate i_r and the expected operational lifespan n :

$$CRF = \frac{i_r(1 + i_r)^n}{(1 + i_r)^n - 1} \quad (S22)$$

The cost balance and auxiliary equations for the components in this study are shown in **Table S1**.

Table S1. Cost and auxiliary equations for each component.

Component	Cost balance equation	Auxiliary equation
ORC Pump	$\dot{C}_2 = \dot{C}_1 + \dot{C}_8 + \dot{Z}_p$	$c_7 = c_8$
Evaporator	$\dot{C}_3 + \dot{C}_{10} = \dot{C}_9 + \dot{C}_2 + \dot{Z}_{ev}$	$c_9 = c_{10}$
Turbine	$\dot{C}_7 + \dot{C}_4 = \dot{C}_3 + \dot{Z}_t$	$c_3 = c_4$
Condenser	$\dot{C}_1 + \dot{C}_6 = \dot{C}_4 + \dot{C}_5 + \dot{Z}_{cn}$	$c_5 = 0$ $c_1 = c_4$
Geothermal well	$\dot{C}_{10} = \dot{Z}_{geo}$	-

The total product cost of the system is given as:

$$\dot{C}_{p,total} = \dot{C}_F + \dot{Z}_{total} = \dot{C}_F + \dot{Z}_{total}^{CI} + \dot{Z}_{total}^{OM} \quad (S23)$$

S2.4. Economic model

Accurate component cost functions are crucial for exergoeconomic analysis. Most studies establish these functions through polynomial fitting on parameters that best characterize each component. The following correlations, based on manufacturing data, are expressed in terms of turbine power output, pump power, and heat exchanger heat transfer area, and provide costs in US dollars.

The above purchase equipment cost (PEC) correlations are adopted from the cited literature and are used in their original cost basis. In the present study, they are applied consistently across all fluids and operating points to enable an internally consistent comparison of economic trade-offs under the same modeling premises. Readers interested

in absolute cost levels should update the PEC values to a common cost year using standard escalation indices (e.g., CEPCI) and local pricing factors, as the simplified correlations and factor method are intended for conceptual-level assessment rather than project-specific cost estimation.

For the working fluid pump of the ORC loop and the water pumps of the other two loops, the PEC can be calculated using[11]:

$$\log_{10}(PEC) = 2.6259 + 1.4395 \log_{10}(\dot{W}_p) + 0.1538(\log_{10}(\dot{W}_p))^2 \quad (S24)$$

Where the pump work, $\dot{W}_p$, is provided in kW.

For the evaporator and condenser, the PEC is calculated using[12]:

$$\log_{10}(PEC) = 4.6656 - 0.1557 \log_{10}(A) + 0.1547(\log_{10}(A))^2 \quad (S25)$$

Where the heat transfer area, A , is provided in m^2 .

For the turbine, the PEC is calculated using[11]:

$$\log_{10}(PEC) = 2.6259 + 1.4395 \log_{10}(\dot{W}_t) - 0.1776(\log_{10}(\dot{W}_t))^2 \quad (S26)$$

Where the Turbine work, $\dot{W}_t$, is provided in kW.

For the geothermal well, the drilling cost is considered as the PEC , which can be a percentage of the total capital investment (TCI), ranging from 25% to 40% for hightemperature plants and 70% for low-temperature plants. The following correlations are used to determine the drilling cost[13]:

$$PEC = \begin{cases} 0.35 \times TCI, & T_g \geq 120^\circ\text{C} \\ 0.7 \times TCI, & T_g < 120^\circ\text{C} \end{cases} \quad (S27)$$

According to Bejan's theory, the TCI for each component is determined as 6.32 times the PEC [9]. As for the operating and maintenance expenses, $\dot{Z}^{om}$, in this study, they are considered as 20% of the PEC [9,11]. This simplified well-cost treatment is used with acceptance at the conceptual level and should be replaced by site- and depth-dependent drilling cost models when the relevant project data are available.

S2.5. Heat exchangers model

The heat exchanger parameters used in this study are provided in **Table S2**. All heat exchangers are assumed to be made of titanium, with a shell and plate type applied to the evaporator and condenser[14]. The heat transfer process is described using the Log Mean Temperature Difference (LMTD) method:

Table S2. Heat exchangers parameters.

Parameter	Value
Type	Shell and plate
Material	Titanium
Flow type	Counter flow
Thickness of the plate t (mm)	0.8
Pitch of the flute p (mm)	1
Depth of the flute a (mm)	1
Thermal conductivity of the plate δ_{he} (W/m K)	17.2
Clearance of the plate γ (mm)	5
Width of the plate w (mm)	605
Number of plates N	200

$$\dot{Q}_k = U_k A_k (LMTD)_k \quad (S28)$$

$$(LMTD)_{ev} = \frac{(T_{10} - T_2) - (T_9 - T_3)}{\log_{10}[(T_{10} - T_2)/(T_9 - T_3)]} \quad (S29)$$

$$(\text{LMTD})_{cn} = \frac{(T_4 - T_6) - (T_1 - T_5)}{\log_{10}[(T_4 - T_6)/(T_1 - T_5)]} \quad (\text{S30})$$

Where U_k is the overall heat transfer coefficient, and A_k is the heat transfer area.

Ignoring the fouling effect, the overall heat transfer coefficient is given by:

$$\frac{1}{U} = \frac{1}{\alpha_{wf}} + \frac{t}{\delta_{hex}} + \frac{1}{\alpha_w} \quad (\text{S31})$$

where α_{wf} and α_w are the convective heat transfer coefficients of the organic working fluid and the secondary loop fluid (geothermal water or cooling water), respectively. t and δ_{hex} are the thickness and thermal conductivity of the heat exchanger plate. The convective heat transfer coefficients can be calculated using the Nusselt number:

$$Nu = \frac{\alpha D_{eq}}{\delta} \quad (\text{S32})$$

Where D_{eq} denotes the equivalent diameter which is approximated to equal twice the clearance of the heat exchanger plate. The following correlations are used to calculate Nusselt number of the water side[15]:

$$Nu_w = 0.04 Re_w^{0.8} Pr_w^{1/3} \quad (\text{S33})$$

Where Re and Pr are Reynolds and Prandtl numbers, which can be calculated with:

$$Re_w = \frac{V_w \cdot D_{eq}}{\nu_w} \quad (\text{S34})$$

$$Pr_w = \frac{cp_w \cdot \mu}{\delta_w} \quad (\text{S35})$$

Where V_w , ν_w , cp_w and μ are the velocity, kinematic viscosity, specific heat capacity, and dynamic viscosity of the water in the heat exchanger channel, respectively. V_w can be calculated from the mass flow rate on the water side:

$$V_w = \frac{\dot{m}_w}{\rho_w \cdot w \cdot \gamma \cdot N} \quad (\text{S36})$$

Where w and N are the width of the heat exchanger plate and the number of plates, respectively.

The following correlation are used to estimate the working fluid boiling heat transfer coefficient at evaporator[14,15]:

$$Nu = \begin{cases} 1.18(f_p X)^{0.919} \cdot H^{-0.834} \cdot \left(\frac{\rho_l}{\rho_v}\right)^{-0.448}, & f_p X \leq 62 \\ 6.646(f_p X)^{0.919} \cdot H^{-0.834} \cdot \left(\frac{\rho_l}{\rho_v}\right)^{-0.448}, & f_p X > 62 \end{cases} \quad (\text{S37})$$

Where f_p is the pressure factor and can be determined by the critical pressure and the atmosphere pressure:

$$f_p = \left[\left(\frac{P}{P_{cr}} \right)^3 + 1 \right] \left(\frac{P}{P_a} \right)^{0.7} \quad (\text{S38})$$

H represents the ratio between sensible heat and latent heat. Moreover, X in the function (S37) is a dimensionless parameter that is calculated as follows:

$$X = \left[\frac{cp_{wf,L} \rho_{wf,L}^2 g}{M^2 N \delta_{wf,L} \sigma L \rho_{wf,v}} \right]^{0.5} D_{eq}^{\frac{3}{2}} q_{ev} \quad (\text{S39})$$

Where M , N is the constant value that are 900 m^{-1} and 1.976 W , respectively.[16,17]

For the convection coefficient at condenser, the following correlation is used;

$$Nu = 2.018 \left(Bo \frac{p^2}{l \cdot a} \right)^{-0.1} \cdot \left(\frac{Gr_L Pr_L}{H} \right)^{\frac{1}{4}} \quad (\text{S40})$$

Where p , l , a are the pitch of the flutes, the heat transfer length and the depth of the flutes, respectively. Bo , Gr are the Bond number and the Grashof number, and can be expressed as:

$$Bo = \frac{g \rho_{wf,L} p^2}{\sigma} \quad (\text{S41})$$

$$Gr = \left(\frac{gl^3}{v_{wf}} \right) \left(\frac{\rho_{wf,L} - \rho_{wf,v}}{\rho_{wf,L}} \right) \quad (S42)$$

Moreover, the following correlations are used to calculate the pressure drop for both sides of heat exchanger:

$$\Delta P_w = F \cdot \frac{\rho_w V_w^2 l}{4w\gamma} \quad (S43)$$

$$\Delta P_{wf} = \frac{2\rho_{wf} V_{wf}^2 l}{D_{eq}} \quad (S44)$$

The flow velocity on the working fluid side can be calculated using an equation in the form of Eq. (S36).

S2.6. Multi-objective optimization model

Multi-objective optimization models are used to solve decision-making problems that involve multiple criteria, allowing for the simultaneous maximization of several objective variables. Unlike single-objective optimization, which results in a single solution, multi-objective optimization yields multiple solutions, referred to as Pareto optimal solutions. Mathematically, the optimization function and constraints can be formulated as follows:

$$\min/\max \quad f_m(x) \quad m = 1, \dots, M \quad (S45)$$

$$\text{s.t.} \quad g_j(x) \leq 0 \quad j=1,\dots,J \quad (S46)$$

$$h_k(x) = 0 \quad k = 1, \dots, K \quad (S47)$$

$$x_i^L \leq x_i \leq x_i^U \quad i = 1, \dots, N \quad (S48)$$

In this study, the optimization objectives are:

1. Maximizing the first law efficiency (η_I).
2. Maximizing the second law efficiency (η_{II}).
3. Maximizing the net power output ($\dot{W}_{net}$).
4. Minimizing the total product cost ($\dot{C}p, total$).
5. Minimizing the total capital investment (TCI).

S2.7. Model validation

To verify the accuracy of the proposed model, data from the literature were used for comparison. The results are shown in **Table S3**.

Table S3. Validation of developed model.

Performance Parameter	Unit	Present work	[2]
$\dot{m}_1$	kg/s	3.53	3.61
$\dot{W}_t$	kW	175.40	180.91
$\dot{W}_{orc,p}$	kW	12.67	13.07
$\dot{Q}_{ev}$	kJ/s	1457.9	1456.85
η_I	%	11.16	11.52
η_{II}	%	35.87	35.05

The derived model shows a maximum deviation of no more than 3.5% compared to the data from the literature. Therefore, the model can be considered reliable.

In the subsequent simulations of this study, the given parameters are listed in the **Table S4** below:

Table S4. Simulation parameters.

Parameter	Value
Environment temperature	15°C

Environment pressure	101.325 kPa
Cooling water temperature	15°C
Geothermal water flow rate	100 kg/s
Pumps isentropic efficiency	95%
urbine isentropic efficiency	89%
Interest rate	5%
Plant economic life	20 years
Annual operating hours	8000 h

S3. Supplementary tables

Table S5. Working fluid candidates considered in the screening stage.

Refrigerant	GWP	OWP	Classification
Ammonia	0	0	Wet
n-pentane	5	0	Dry
Isobutane	3	0	Dry
R11	4750	1	Isentropic
R113	6130	0.85	Dry
R1224yd(Z)	1	0	Dry
R123	77	0.01	Dry
R1233zd(E)	1	0	Dry
R1234ze(E)	<1	0	Isentropic
R1234ze(Z)	<1	0	Isentropic
R134a(Z)	1430	0	Wet
R141b	725	0.12	Dry
R152a	124	0	Wet
R227ea	3220	0	Dry
R236ea	1410	0	Dry
R236fa	9810	0	Dry
R245ca	726	0	Dry
R245fa	1030	0	Dry
R600	4	0	Dry

Table S6. ORC orthogonal experiment.

No.	Factors					
	A (kg/s)	B (t/h)	C (t/h)	D (°C)	E (°C)	F (kW)
1	0.3	7	12	80	20	21
2	0.3	10.25	25	102.5	40	24
3	0.3	13.5	38	87.5	35	27
4	0.3	16.75	18.5	110	30	30
5	0.3	20	31.5	95	25	21
6	0.53	7	38	102.5	30	24
7	0.53	10.25	18.5	87.5	25	21
8	0.53	13.5	31.5	110	20	24

9	0.53	16.75	12	95	40	27
10	0.53	20	25	80	35	30
11	0.75	7	31.5	87.5	40	30
12	0.75	10.25	12	110	35	27
13	0.75	13.5	25	95	30	21
14	0.75	16.75	38	80	25	24
15	0.75	20	18.5	102.5	20	27
16	0.97	7	25	110	25	27
17	0.97	10.25	38	95	20	30
18	0.97	13.5	18.5	80	40	30
19	0.97	16.75	31.5	102.5	35	21
20	0.97	20	12	87.5	30	24
21	1.2	7	18.5	95	35	24
22	1.2	10.25	31.5	80	30	27
23	1.2	13.5	12	102.5	25	30
24	1.2	16.75	38	110	20	21
25	1.2	20	25	87.5	40	21

Table S7 Instrumentation and measured variables for the 20 kW ORC rig (Case I). Measurement locations are indicated in Figure 6 using the same point labels (P1–P13, T1–T12).

Category	Measured variable	Location
Flow rates	Working-fluid loop flow rate	Working-fluid loop flow meter
	Hot-water (heat-source) loop flow rate	Heat-source water loop
	Cooling-water loop flow rate	Cooling-water loop
Pressures	Pressure at P1–P13	Pressure taps at labeled points P1–P13 in Figure 6
Temperatures	Temperature at T1–T12	Temperature sensors at labeled points T1–T12 in Figure 6
	Heating-water tank temperature	Heating-water tank
Control signals	Main-loop valve opening	Valve position feedback
	Expander inlet valve opening	Valve position feedback
	Bypass valve opening	Valve position feedback
Pump drives	Working-fluid pump frequency	Pump drive signal
	Hot-water pump frequency	Pump drive signal
	Cooling-water pump frequency	Pump drive signal

Rotating machinery	Expander-generator rotational speed	Speed sensor
	Load-bank voltage	Resistive load bank
Electrical/load	Load-bank current	Resistive load bank
	Active power (phase / total)	Resistive load bank
	Electrical frequency	Resistive load bank
Condition monitoring	Vibration (expander inlet)	Vibration sensor
	Vibration (expander outlet)	Vibration sensor
	Gas detector reading	Gas detector
	Tank liquid level	Level sensor
Auxiliary	Auxiliary channel temperatures (CH1–CH5)	Auxiliary temperature channels

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