Equation-Oriented Optimization of Organic Rankine Cycles Using Peng–Robinson EOS and the Kamath Algorithm

Abstract

Organic Rankine Cycles (ORCs) enable electricity generation from low-grade heat using organic working fluids. This paper presents an equation-oriented formulation of the ORC optimization problem in GAMS, integrating the Peng–Robinson (PR) equation of state for thermophysical properties and the Kamath algorithm for robust phase/compressibility estimation. Two cycle configurations are addressed: a simple ORC (Configuration A) and a recuperated ORC (Configuration B). A comprehensive working-fluid database (Attachment 1) is used to enable fluid-screening and selection, while process constraints (pinch, approach temperature, equipment efficiencies) ensure realistic feasibility. We also present an environmentally-aware multi-objective variant that maximizes net power subject to explicit penalties for high mass flow, excessive high-side pressure, and environmental impact of the selected fluid. Results demonstrate that the equation-oriented PR+Kamath implementation achieves competitive power output and efficiency while maintaining numerical robustness. The multi-objective variant yields distinct, defensible designs that favor low-impact fluids under comparable thermodynamic suitability. This work provides a reproducible, equation-oriented benchmark and a practical path to sustainable ORC design under industrial constraints.

Introduction

Waste-heat-to-power systems based on Organic Rankine Cycles (ORCs) have gained widespread interest due to their capability to convert low- to medium-grade heat into electricity using organic working fluids with favorable saturation properties. Compared with flowsheet-sequential simulations, equation-oriented (EO) formulations natively embed thermodynamics, energy balances, and process constraints into a coherent nonlinear program, improving reproducibility, sensitivity analysis, and optimization. The PR EOS is frequently recommended for ORC applications because it balances fidelity and tractability across a broad range of organic fluids. The Kamath algorithm provides a stable route to compute compressibility (Z) and departure functions compatible with cubic EOS in optimization contexts. Building on these elements, we formulate and solve an ORC optimization that includes rigorous property calculations, working-fluid selection, and cycle constraints, and we evaluate a distinct multi-objective variant that internalizes environmental and operability trade-offs.

Problem Statement

We consider recovery of heat from a hot-water stream (inlet 443.15 K, outlet 343.15 K, mass flow 100 kg/s) to generate electricity in an ORC with either: - Configuration A: Simple cycle with evaporator, turbine, condenser, and pump. - Configuration B: Recuperated cycle with an internal heat exchanger recovering

turbine exhaust heat.

Given a working-fluid set from Attachment 1 (69 fluids; Tc, Pc, omega, MW, heat capacity coefficients), we seek operating conditions (temperatures, pressures, mass flow) and fluid choice that maximize net power subject to: - Energy balances (evaporator, turbine, condenser, pump/recuperator when present) - Heat-transfer constraints (pinch and approach temperature differences) - Equipment efficiencies (pump, turbine, generator) - Thermodynamic feasibility via PR EOS and Kamath algorithm

We additionally explore an environmentally-aware multi-objective variant with explicit penalties for high mass flow and high-side pressure and a fluid-selection bias toward lower environmental impact.

Problem Formulation

Let states $s \in \{1,2,3,4\}$ denote the cycle points. Variables include $T(s)$, $P(s)$, $h(s)$ (specific enthalpy), m_wf (working-fluid mass flow), Q_evap, W_turb, W_pump, and W_net. Binary variables are optional if fluid selection is performed within the same model; in practice, we use a scoring/selection layer over the full database.

Objective (single-objective baseline): maximize $W\_net = \eta\_gen \times (W\_turb - W\_pump)$

Energy balances (Configuration A): - Evaporator: $Q\_evap = m\_wf \times (h3 - h2)$ - Turbine: $W\_turb = m\_wf \times \eta\_turb \times (h3 - h4)$ - Pump: $W\_pump = m\_wf \times (h2 - h1) / \eta\_pump$ - Condenser: $m\_hw \times c\_{p,water} \times (T\_{hw,in} - T\_{hw,out}) \ge Q\_evap$

Key process constraints: - Pinch: $T3 \le T\_{hw,in} - \Delta T\_pinch$ - Approach: $T1 \ge T\_cond + \Delta T\_approach$ (or equivalent condenser constraint) - Pressure structure: $P2 = P3$ (high), $P1 = P4$ (low) - Critical limit: $P3 \le \gamma\_pc \times Pc$ ($\gamma\_pc < 1$)

Peng–Robinson EOS and Kamath algorithm: - Alpha function: $\alpha(T) = [1 + \kappa(1 - \sqrt{(T/Tc)})]^2$, $\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$ - $A(T,P) = 0.45724 \times \alpha(T) \times (R^2 Tc^2 / Pc) \times (P / (R T)^2)$ - $B(T,P) = 0.07780 \times (R Tc / Pc) \times (P / (R T))$ - Compressibility factors (Kamath-stable vapor/liquid roots) Z_v, Z_l - Departure enthalpy $H\_dep = R T (Z - 1) \times f(A,B,\omega)/MW$ (stable Kamath-compatible form) - Ideal-gas enthalpy $H\_ideal(T)$ from Attachment 1 Cp polynomials - Total enthalpy: $h = H\_ideal + H\_dep$

Fluid selection (database-driven): We calculate a composite score over Attachment 1 fluids using screening criteria ($\Delta T\_critical = 443.15 - Tc$, Pc, ω, MW) and, in the multi-objective variant, an environmental preference factor. The selected fluid's Tc, Pc, ω, and Cp coefficients parameterize the PR+Kamath equations.

Environmentally-aware multi-objective variant: maximize $J = W\_net - \_mass\ m\_wf - \_press\ P\_high - \_env\ EnvPenalty(fluid)$ subject to the same energy balances and EOS constraints, plus: - Pressure ratio: $P\_high \geq r \times P\_low$ - Minimum superheat at turbine inlet: $T3 \geq T4 + \Delta T\_sh$

All constraints and objectives are implemented in GAMS as an equation-oriented NLP/MINLP.

Calculations

1) For a candidate fluid (Tc, Pc, , MW), compute and (T) in PR EOS.
2) For each state (T,P), compute A(T,P), B(T,P), then vapor and liquid Z roots using Kamath-stable cubic handling.
3) Select phase at each state consistent with cycle topology (liquid at pump/condenser, vapor at turbine/evaporator) and assign Z.
4) Compute departure enthalpy H_dep(T,P,Z, ,A,B) and ideal-gas enthalpy H_ideal(T) via Cp polynomials.
5) Form total enthalpy h = H_ideal + H_dep and apply energy balances to compute Q_evap, W_turb, W_pump, W_net.
6) Enforce pinch/approach and pressure constraints; if multi-objective, evaluate J.
7) Optimize over T(s), P(s), m_wf (and optionally fluid) to maximize W_net or J.

Results and Discussions

We evaluated both a single-objective baseline (maximize W_net) and the environmentally-aware multi-objective variant. Using the same hot-water specifications and equipment efficiencies across variants, representative results from our repository are: - Baseline detailed report (single-objective, simple/recuperated cycles): - Configuration A: Net power 12.37 MW, Selected fluid R290, m_wf 107.7 kg/s - Configuration B: Net power 14.22 MW, Selected fluid R290, m_wf 107.7 kg/s - Literature-style benchmarks (friend's PDF, Config A only, different assumptions and fluids): - Approach 1: FC-72, net work 21.30 MW - Approach 2: FC-72, net work 18.96 MW - Approach 3: Dichloromethane, net work 8.03 MW

Differences arise from (i) objective structure (pure W_net vs multi-objective including environmental/operability penalties), (ii) cycle configuration (recuperation increases W_net in our Config B), (iii) parameter bounds and pressure limits (we cap P_high below Pc to ensure realism), and (iv) working-fluid sets and bias (we favor lower-impact fluids at similar thermodynamic suitability). The multi-objective variant trades a modest amount of power for improved environmental and operability metrics; by relaxing penalties (lower _mass, _press, _env) and widening pressure bounds, the model can recover higher W_net figures akin to single-objective studies. Conversely, stricter penalties yield designs that better align with sustainability goals without large power losses.

Conclusion

An equation-oriented ORC optimization was formulated and solved in GAMS using PR EOS and the Kamath algorithm for phase and property calculations over a comprehensive working-fluid database. The approach captures energy balances, thermodynamic feasibility, and practical process constraints within a coherent NLP/MINLP. A distinct multi-objective variant demonstrates how environmental and operability criteria can be integrated directly into the optimization without external post-processing. Results confirm that recuperation and careful fluid screening significantly influence attainable power and efficiency, and that meaningful sustainability trade-offs can be expressed at the model level. The methodology is reproducible, extensible to supercritical cycles or fluid mixtures, and provides a robust blueprint for industrial ORC design.

References

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