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 {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 = _gen × (W_turb − W_pump)

Energy balances (Configuration A): - Evaporator: Q_evap = m_wf × (h3 − h2) - Turbine: W_turb = m_wf × _turb × (h3 − h4) - Pump: W_pump = m_wf × (h2 − h1) / _pump - Condenser: m_hw × c_p,water × (T_hw,in − T_hw,out) Q_evap

Key process constraints: - Pinch: T3 T_hw,in − ΔT_pinch - Approach: T1 T_cond + ΔT_approach (or equivalent condenser constraint) - Pressure structure: P2 = P3 (high), P1 = P4 (low) - Critical limit: P3 _pc × Pc (_pc < 1)

Peng–Robinson EOS and Kamath algorithm: - Alpha function: (T) = [1 + (1 − √(T/Tc))]^2, = 0.37464 + 1.54226 − 0.26992 ^2 - A(T,P) = 0.45724 × (T) × (R^2 Tc^2 / Pc) × (P / (R T)^2) - B(T,P) = 0.07780 × (R Tc / Pc) × (P / (R T)) - Compressibility factors (Kamath-stable vapor/liquid roots) Z_v, Z_l - Departure enthalpy H_dep = R T (Z − 1) × f(A,B,)/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 (ΔT_critical = 443.15 − Tc, Pc, , MW) and, in the multi-objective variant, an environmental preference factor. The selected fluid's Tc, Pc, , 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 r × P_low - Minimum superheat at turbine inlet: T3 T4 + ΔT_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 assessed two equation-oriented formulations: (i) a single-objective baseline that maximizes net power (W_net) and (ii) an environmentally-aware multi-objective variant that penalizes high working-fluid flow, excessive high-side pressure, and environmentally unfavorable fluids. Unless noted, the hot-water conditions and equipment efficiencies are identical across runs.

Core results from the baseline model (repository detailed report): - Configuration A (simple ORC): - Net power: 12.37 MW - Selected working fluid: R290 - Working-fluid mass flow: 107.7 kg/s - Configuration B (recuperated ORC): - Net power: 14.22 MW - Selected working fluid: R290 - Working-fluid mass flow: 107.7 kg/s

Interpretation: - At identical source/sink conditions, recuperation increases the available temperature glide for preheating the working fluid, reducing external heat demand and improving the cycle's net work (+1.85 MW vs Configuration A). - R290 appears as a robust choice for both configurations under the stated bounds, reflecting an adequate balance of critical properties (Tc, Pc) and acentric factor for the specified condenser and evaporator targets.

Effect of objective structure (multi-objective variant): - When modest penalty weights are introduced (_mass, _press, _env), the optimizer shifts towards solutions with lower high-side pressure and reduced working-fluid flow, typically sacrificing a small fraction of W_net while improving operational headroom and environmental preference. - Reducing penalty weights or relaxing pressure bounds shifts the solution back towards the single-objective outcome (higher W_net, larger m_wf, and higher P_high). This controllable trade-off allows tailoring the design to site priorities (pure power vs. sustainability/safety margins).

Robustness and model fidelity: - The PR EOS with Kamath's cubic handling provided stable compressibility factors and departure enthalpies across all state points, enabling consistent energy balances in both configurations. - Practical bounds on pressure relative to critical pressure (P_high _pc Pc) prevent unrealistic operation near the critical region while still allowing competitive power.

Design implications: - If the project prioritizes maximum power at fixed source/sink conditions, the baseline formulation with recuperation is preferred. - If safety, equipment cost, or environmental impact must be weighted explicitly, the multi-objective formulation offers a principled lever to trade a modest amount of power for lower P_high, reduced m_wf, and more sustainable fluid choices.

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.

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