# Problem Statement and Problem Formulation (Equation-Oriented, PR EOS + Kamath)

## Problem Statement (<= 1000 words)

Objective - We aim to convert low- to medium-grade waste heat into electricity using an Organic Rankine Cycle (ORC) under industrially realistic constraints, and to formulate the optimization in an equation-oriented (EO) manner suitable for rigorous solution.

Scope and configurations - 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

Given data (nominal)

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

| Item | Symbol | Value | Units |
| --- | --- | --- | --- |
| Hot-water inlet temperature | T\_hw\_in | 443.15 | K |
| Hot-water outlet temperature | T\_hw\_out | 343.15 | K |
| Hot-water mass flow | m\_hot | 100 | kg/s |
| Water heat capacity | Cp\_water | 4.18 | kJ/(kg\*K) |
| Condenser approach | dT\_approach | 5 | K |
| Evaporator pinch | dT\_pinch | 5 | K |
| Pump isentropic efficiency | eta\_pump | 0.75 | - |
| Turbine isentropic efficiency | eta\_turb | 0.80 | - |
| Generator efficiency | eta\_gen | 0.95 | - |

Working-fluid candidates and selection (pure fluids) - 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.

Decision levers - Operating variables: state temperatures T(s) and pressures P(s) at the cycle points; working-fluid mass flow m\_wf. - Working-fluid identity: chosen from the candidate set (exactly one pure fluid active). - Recuperator (Configuration B): internal duty and pinch.

Performance targets - Maximize net electrical power while satisfying process and thermodynamic constraints. - Primary focus on Configuration A per assignment; Configuration B is treated as an optional extension. - Optionally explore trade-offs (e.g., operating conservatism) with a composite objective.

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 the same approach as the model code: Cp(T) polynomials if present, otherwise a constant cp\_avg. Total enthalpy is H = H\_ideal(T) + H\_departure(T,P,Z).

Assumptions - Steady state; single working fluid per case; negligible heat losses outside modeled exchangers; pressure drops lumped into equipment where applicable. - PR EOS provides adequate accuracy over the operating window; Cp(T) polynomials are valid in the temperature range of interest. - Ambient conditions remain fixed for condenser approach evaluation.

Key outputs - Net power W\_net, thermal efficiency, specific work, working-fluid mass flow, high/low pressures, state temperatures, and (for Configuration B) recuperator duty and internal pinch.

Validation note - 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\_turb and W\_net.

## Problem Formulation (<= 1000 words)

Sets and states - We use a four-state numbering for the simple cycle: - 1: condenser outlet (low pressure, liquid) - 2: pump outlet (high pressure, liquid) - 3: evaporator outlet (high pressure, vapor) - 4: turbine outlet (low pressure, vapor) - For the recuperated cycle, we add two states: - 5: recuperator hot outlet (low pressure, cooled vapor) - 6: recuperator cold outlet (high pressure, preheated liquid)

Decision variables - T(s) [K], P(s) [bar], Z(s) [-], H\_ideal(s) [kJ/kg], H\_dep(s) [kJ/kg], H(s) [kJ/kg] - m\_wf [kg/s], Q\_evap [kW], Q\_recup [kW], W\_pump [kW], W\_turb [kW], W\_net [kW] - Fluid selection dof: either binary indicators y\_i (sum\_i y\_i = 1) for an integrated selection, or an external screening step that activates one pure fluid per run.

Objective (baseline) - Maximize net power:

Energy balances and duties

Isentropic relations (engineering form) - Turbine (3 -> 4):

- Pump (1 -> 2):

- Here k = cp / (cp - R\_spec) and cp(T) is obtained from the derivative of H\_ideal(T). - Note: A full PR-based isentropic step would use s-const constraints; the above is a robust approximation that preserves units and trends without introducing additional differential relations.

Heat-transfer and pressure-structure constraints

Recuperator constraints (Configuration B)

Thermodynamics: PR EOS and enthalpy model

- Phase consistency: use Z\_liquid downstream of condenser/pump, Z\_vapor downstream of evaporator/turbine. - Units: H in kJ/kg, m\_wf in kg/s, hence powers in kW by construction.

Variable bounds (illustrative)

300 <= T(1) <= 370 ; K  
300 <= T(2) <= 390  
360 <= T(3) <= T\_hw\_in - dT\_pinch  
300 <= T(4) <= 420  
1 <= P(s) <= 0.75\*Pc ; bar  
1 <= m\_wf <= 120 ; kg/s

Optional multi-objective extension

- Nonnegative weights encode preferences for lower flow (smaller equipment) and lower high-side pressure (operability/safety).

Reporting and comparison - We present tabulated results for A and B: W\_pump, W\_turb, W\_net, m\_wf, key temperatures/pressures; for B, we also include Q\_recup and internal pinch. When comparing with flowsheet simulations, we ensure matched boundary conditions and the same working fluid to avoid misleading differences.

Model-specific symbols (for clarity) - component: index over pure working fluids (at least five candidates) - properties: columns for Tc, Pc, omega, MW, Tb, density, h\_form, h\_vap (units: consistent with the enthalpy basis) - coefficient: Cp(T) polynomial coefficients a..f (for H\_ideal(T) integration) - y(component): pure-fluid selector (sum y = 1) - Selected properties: Tc, Pc, omega, MW via y-weighted sums - R\_spec = 8.314 / MW (kJ/kg/K); Cp per kg = Cp\_kmol / MW