# 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 pressure | P\_hw | 10 | bara |
| 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 |
| Cooling air inlet temperature | T\_air\_in | 298.15 | K (25 °C) |
| Water heat capacity | Cp\_water | 4.675 | 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 (optional extension).

### 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 cp\_avg. Total enthalpy is H = H\_ideal(T) + H\_departure(T,P,Z).

### Assumptions

* Steady state; negligible heat losses outside modeled exchangers; pressure drops in exchangers per Table 2; ambient conditions fixed for condenser approach.

### 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 (core form):

If a stabilization/selection penalty is used in the implementation, the objective is written as:

where is a large coefficient (Big-M–style) and are the vapor/liquid indicators at state 2 used to enforce consistent phase selection. When the penalty is inactive (recommended for reporting), equation (1) is used.

### Energy balances and duties

Explanation: Baseline thermodynamic identity; in MMMMMM.gms a head-based form (4’) is used. Implementation in MMMMMM.gms (head-based pump work):

### Isentropic relations (engineering form)

Explanation: Reference equations often used in EO modeling; not enforced in MMMMMM.gms. - 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.

Implementation status in MMMMMM.gms: - The explicit isentropic T-relations (6)–(7) are not enforced in the current MMMMMM.gms. - The turbine efficiency parameter is defined but not applied; turbine work uses enthalpy difference as in (3). - Pump work follows the head-based expression (4’).

### Heat-transfer and pressure-structure constraints

Explanation: These constraints encode minimum temperature driving forces and the high/low pressure structure; (11) keeps operation below critical pressure to avoid pathological regions.

### Recuperator constraints (Configuration B)

Explanation: Energy balance equates hot- and cold-side duties; minimum approach prevents temperature cross and ensures feasible heat exchange.

### 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. Explanation: PR EOS gives Z and departure enthalpy; Kamath-compatible root handling ensures stable liquid/vapor roots for Z in optimization.

### 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

Explanation: Bounds reflect physical feasibility and help the NLP avoid nonphysical regions (e.g., near-critical pressures, sub-ambient temperatures).

### Optional multi-objective extension

- Nonnegative weights encode preferences for lower flow (smaller equipment) and lower high-side pressure (operability/safety). Explanation: Penalizing flow and P\_high trades a small portion of power for improved operability and downsized equipment.

### 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