# Problem Statement and Problem Formulation (EO GAMS, PR EOS + Kamath)

## Problem Statement (<= 1000 words)

Objective - Convert low- to medium-grade waste heat into electricity using an Organic Rankine Cycle (ORC) under industrially realistic constraints, and formulate the optimization in an equation-oriented (EO) manner suitable for direct solution in GAMS. - Implementation reference: the EO model is implemented in the GAMS file “MMMMMM.gms” (all symbols and equations below follow the same naming convention in that file).

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)

| 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 database (Attachment 1) - Each candidate working fluid provides: critical temperature Tc, critical pressure Pc, acentric factor omega, molecular weight MW, and ideal-gas heat capacity coefficients Cp(T) as a polynomial in T.

Decision levers (mapped 1:1 to MMMMMM.gms) - Operating variables: state temperatures T(s) and pressures P(s) at the cycle points; working-fluid mass flow m\_wf. - Working-fluid identity: selected from the database based on thermodynamic screening and optimization. - Recuperator (Configuration B): internal duty and pinch.

Performance targets - Maximize net electrical power while satisfying process and thermodynamic constraints. - Compare architectures (A vs B) on a like-for-like basis. - Optionally explore trade-offs (e.g., operating conservatism or environmental preference) with a multi-objective 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 is computed from Cp(T) polynomials; total enthalpy is H = H\_ideal(T) + H\_departure(T,P,Z).

Assumptions - Steady state; single working fluid per run; 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, selected fluid, high/low pressures, state temperatures, and (for Configuration B) recuperator duty and internal pinch.

Validation note - For fair EO–HYSYS comparisons, both models must use matched boundary conditions (source/sink), identical fluid identity and property package, and consistent unit systems. Differences in fluid choice, bounds, or property methods can materially change W\_turb and W\_net. - Practical tip: when reporting or debugging, cite values from MMMMMM.gms run logs (W\_turb, W\_pump, W\_net, Q\_evap) to ensure consistency with this section.

## Problem Formulation (<= 1000 words)

Sets and states - 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, add states: - 5: recuperator hot outlet (low pressure, cooled vapor) - 6: recuperator cold outlet (high pressure, preheated liquid)

Decision variables (as declared in MMMMMM.gms) - 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]

Objective (baseline) - Maximize net power:

W\_net = eta\_gen \* ( W\_turb - W\_pump )

* This objective is coded as the net power equation in MMMMMM.gms (see NET POWER block).

Energy balances and duties (equation names in MMMMMM.gms mirror these relations)

Q\_evap = m\_wf \* ( H(3) - H(2) ) ; simple A  
Q\_evap = m\_wf \* ( H(3) - H(6) ) ; recuperated B  
W\_turb = m\_wf \* ( H(3) - H(4) )  
W\_pump = m\_wf \* ( H(2) - H(1) )  
  
m\_hot \* Cp\_water \* ( T\_hw\_in - T\_hw\_out ) >= Q\_evap

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

T4s = T3 \* ( P4 / P3 )^((k3 - 1)/k3) ; polytropic ideal-gas approx.  
T4 = T3 - eta\_turb \* ( T3 - T4s )

* Pump (1 -> 2):

T2s = T1 \* ( P2 / P1 )^((k1 - 1)/k1)  
T2 = T1 + ( T2s - T1 ) / eta\_pump

* 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

T(3) <= T\_hw\_in - dT\_pinch ; evaporator pinch  
T(1) >= T\_cond + dT\_approach ; condenser approach (T\_cond from site)  
P(2) = P(3) ; high pressure  
P(1) = P(4) ; low pressure  
P(3) <= alpha\_pc \* Pc ; critical-pressure cap (0 < alpha\_pc < 1)

Recuperator constraints (Configuration B)

m\_wf \* ( H(4) - H(5) ) = m\_wf \* ( H(6) - H(2) )  
T(4) - T(6) >= dT\_recup ; hot end pinch  
T(5) - T(2) >= dT\_recup ; cold end pinch

Thermodynamics: PR EOS and enthalpy model

alpha(T) = [ 1 + kappa \* ( 1 - sqrt( T / Tc ) ) ]^2  
kappa = 0.37464 + 1.54226\*omega - 0.26992\*omega^2  
  
A = 0.45724 \* (R\_bar^2 \* Tc^2 / Pc) \* alpha(T) \* P / (R\_bar\*T)^2  
B = 0.07780 \* (R\_bar \* Tc / Pc) \* P / (R\_bar\*T)  
  
Z\_vapor = 1 + B + A\*B/(3 + 2\*B)  
Z\_liquid = B + A\*B/(2 + 3\*B)  
  
H\_ideal(T) = integral Cp(T) dT from T\_ref to T ; Cp polynomials from DB  
H\_dep(T,P,Z) = R\_spec \* T \* ( Z - 1 ) ; robust departure form  
H(T,P) = H\_ideal(T) + H\_dep(T,P,Z)

* 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; use the same ranges in MMMMMM.gms)

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

Maximize J = W\_net - lambda\_mass \* m\_wf - lambda\_press \* P(3) - lambda\_env \* EnvPenalty(fluid)

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

Reporting and comparison - Present tabulated results for A and B: W\_pump, W\_turb, W\_net, m\_wf, selected fluid, key temperatures/pressures. For B, include Q\_recup and internal pinch. - When comparing with HYSYS, ensure matched boundary conditions and fluid identity; otherwise, differences in W\_turb and W\_net are expected.