

Article

Thermodynamic Optimization of a Combined Cycle Cogeneration System for Petroleum Refinery Applications

Martín Salazar-Pereyra ¹, Ladislao Eduardo Méndez-Cruz ¹, Wenceslao Bonilla-Blancas ¹, Raúl Lugo-Leyte ², Sergio Castro-Hernández ² and Helen D. Lugo-Méndez ^{3,*}

¹ Tecnológico Nacional de México/TES de Ecatepec, Av. Tecnológico S/N, Col. Valle de Anáhuac, Ecatepec de Morelos 55210, Mexico; msalazar@tese.edu.mx (M.S.-P.); wcbonilla@tese.edu.mx (W.B.-B.)

² Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana—Iztapalapa, Av. Ferrocarril San Rafael Atlixco No. 186, Colonia Leyes de Reforma 1ª Sección, Iztapalapa, Mexico City 09340, Mexico; sch@xanum.uam.mx (S.C.-H.)

³ Departamento de Procesos y Tecnología, Universidad Autónoma Metropolitana—Cuajimalpa, Av. Vasco de Quiroga No. 4871, Colonia Santa Fé, Cuajimalpa, Mexico City 05348, Mexico

* Correspondence: hlugo@cua.uam.mx

Abstract

Cogeneration system optimization in refineries confronts the challenge of simultaneously integrating design parameter selection and topological configuration. The literature typically addresses these aspects separately: parametric optimization with fixed topology or configuration optimization for specific nominal conditions. This work develops a comprehensive methodology integrating exhaustive parametric exploration with superstructure-based optimization through mixed-integer nonlinear programming (MINLP), applied to the Miguel Hidalgo refinery in Tula, Mexico. The systematic procedure generates superstructures considering all viable expansion and tempering routes under steam quality restrictions ($x \geq 0.88$), evaluating 84–105 combinations of generation pressure ($P_{\text{HRSG}} = 70\text{--}140$ bar) and superheater outlet temperature ($T_{s4} = 500\text{--}560$ °C). The analysis reveals three topologically distinct configurations identified as generating maximum power under different operating conditions and characterizes how transitions between high-performing configurations occur at discrete thermodynamic thresholds that correlate with constraint activation contradicting the conventional assumption of continuous parameter-configuration relationships. Multi-criteria evaluation positions Configuration 1 as the recommended design, generating 25% increase in electric generation, 11% improvement in utilization factor (UF : $0.640 \rightarrow 0.710$) and 20% reduction in specific fuel consumption (SFC : $0.259 \rightarrow 0.207$ kg/kWh). The methodology is directly generalizable to other refineries through universal thermodynamic principles, with a systematic five-step procedure applicable to any multi-pressure steam demand profile. The characterization of discrete transition phenomena and the associated methodology for their thermodynamic explanation challenges the conventional assumption of continuous parameter-configuration relationships in optimization approaches, with immediate implications for the design of flexible cogeneration systems in refineries worldwide.

Keywords: cogeneration; superstructure optimization; MINLP; petroleum refineries; combined cycle; parametric analysis; discrete topology transitions; thermodynamic mechanisms; industrial implementation; PEMEX



Academic Editors: Muhammad Faizan Tahir, Luca Cimmino and Francesco Calise

Received: 28 January 2026

Revised: 13 March 2026

Accepted: 18 March 2026

Published: 23 March 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article

distributed under the terms and

conditions of the [Creative Commons](https://creativecommons.org/licenses/by/4.0/)

[Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

1. Introduction

Petroleum refineries represent energy-intensive industrial facilities that simultaneously demand electricity and process steam at multiple pressure levels for hydrotreatment, distillation, and catalytic reforming operations [1,2]. The conventional configuration—steam generation in boilers through direct combustion (thermal efficiency 80–85%) and electricity supply from the national grid—results in inefficient utilization of primary energy. Cogeneration systems based on gas turbines with heat recovery steam generators (HRSGs) and integrated steam cycles can achieve overall fuel utilization efficiencies of 70–85% [1,3,4], representing a critical strategy for fuel consumption and CO₂ emissions reduction in the industrial sector [5]. The literature consistently documents operating cost reductions of 15–20% [6,7], emissions decreases of 20–30% [8,9], and payback periods of 2–4 years for large-scale applications.

The literature on cogeneration optimization in refineries can be classified into three methodological approaches. The first evaluates specific predefined configurations through detailed thermodynamic simulation. Costea and Feidt [3] demonstrated efficiencies of 75–85% in multi-pressure combined cycles, while Mehrpooya et al. [4] quantified 12–15% reductions in specific fuel consumption. Pariasamy et al. [10] reviewed refinery configurations, documenting decreases in generation costs. These works report significant improvements but typically analyze a topology selected a priori, limiting the search space. The second approach addresses operational optimization for systems with fixed topology. Chen et al. [6] developed comprehensive MINLP models for retrofit, distinguishing three contexts: operational optimization (3–5% improvements), retrofit with restricted modifications (12–18% improvements), and greenfield design with free topology. Manesh et al. [9] and Lazzaretto and Toffolo [11,12] developed thermoeconomic optimization methodologies. A common characteristic is that these studies typically fix HRSG design parameters at nominal values, then optimize configuration for that specific point [13,14]. The third approach uses mixed-integer programming (MINLP) for simultaneous topology synthesis through superstructures [15,16]. Variny et al. [17] optimized systems with 15 pressure levels, Martelli et al. [18] proposed master–slave decomposition, Marty et al. [19] designed organic Rankine cycles with automated fluid selection. However, each implementation focuses on a specific system with ad hoc-derived superstructure, without guaranteeing the consideration of all thermodynamically viable alternatives [20,21].

Despite the progress in superstructure-based optimization, there exists an unresolved methodological tension between systematic parametric exploration and topological optimization. Existing studies typically adopt one of two approaches: (1) fixing HRSG design parameters at nominal values and optimize topology for those conditions or (2) optimizing operational parameters for a predefined topological configuration. Systematic exploration of the two-dimensional space (design parameters × optimal topology) remains scarcely reported in the refinery cogeneration literature. This gap limits understanding of how nonlinear thermodynamic constraints—particularly the minimum steam quality constraint ($x \geq 0.88$) to prevent blade erosion [22,23]—can induce discrete transitions between optimal configurations when operational parameters cross critical thresholds.

The optimization of cogeneration systems in refineries has advanced significantly through superstructure-based approaches, which systematically integrate multiple technologies using mathematical models such as MILP and MINLP to explore alternative configurations [24,25]. These models traditionally organize units in a hierarchical series–parallel process network but may present limitations in faithfully representing critical nonlinear relationships, such as thermodynamic properties or steam quality constraints in steam turbines [26]. Although recent studies have incorporated rigorous correlations and propositional logic to exclude infeasible configurations, and have even addressed specific

problems such as hydrogen management through MINLP superstructures [27], the simultaneous exploration of parametric and topological spaces in cogeneration remains a challenge due to strong nonlinearities and the presence of integer variables. Moreover, phenomena such as abrupt shifts between optimal configurations under variations in product prices or operating conditions, observed in optimization under uncertainty in other energy sectors, have not been sufficiently examined in the refinery context, where thermodynamic and economic constraints can induce discrete changes in the selected topology.

This work identifies three specific limitations. First, topological preselection approaches limit the search space without a systematic completeness guarantee [20]. Second, optimization for specific HRSG nominal conditions is insufficient for greenfield projects where freedom exists to specify parameters; sensitivity of optimal configurations to parametric variations remains scarcely characterized [6,13]. Third, the implicit assumption of continuity between parameters and optimal configuration lacks explicit verification; active thermodynamic constraints can induce discrete transitions when parameters cross thresholds, a phenomenon not systematically documented.

The present work applies to the cogeneration project between the Federal Electricity Commission (CFE) and Mexican Petroleum (PEMEX) at the Miguel Hidalgo refinery, Tula, Hidalgo. This project forms part of the national strategy for energy efficiency and refinery modernization. Four out-of-service gas turbines will be rehabilitated for simultaneous generation of electricity and process steam through cogeneration. This case represents an appropriate context for methodological research by combining typical refinery characteristics with design freedom for specification of rehabilitated HRSG parameters.

This work addresses the following research question: how does the optimal steam cycle configuration vary with fundamental HRSG operational parameters, and what thermodynamic mechanisms cause transitions between configurations? Specifically, it seeks to: (1) develop a systematic procedure for superstructure construction that guarantees consideration of all thermodynamically viable alternatives; (2) quantify performance sensitivity to pressure and HRSG temperature variations, identifying high-sensitivity regions versus robust zones; and (3) characterize mechanisms causing discrete transitions between configurations, determining whether they occur at predictable thresholds through a priori thermodynamic analysis.

The main contributions are organized into three categories. Methodologically, a systematic four-step procedure for superstructure construction is developed: (1) identification of relevant pressure levels, (2) thermodynamic viability evaluation through quality criterion $x \geq 0.88$, (3) definition of multi-stage turbines for viable routes, and (4) integration into complete superstructure with formal completeness verification. A rigorous MINLP model incorporating mass and energy balances, steam quality constraints, and technological limits is formulated, being directly transferable to other facilities through specification of particular demands. Scientifically, distinct optimal configurations emerging under different HRSG conditions are identified, demonstrating optimal topology dependence on design parameters. A phenomenon of discrete transitions induced by quality constraint when parameters cross critical thresholds determined by energy balances in mixers is discovered. Thermodynamic analysis explaining causal physical mechanisms is developed, allowing anticipation of transition thresholds. Performance surfaces in two-dimensional parametric space are quantified (pressure $P_{\text{HRSG}} = 75\text{--}140$ bar, temperature $T_{s4} = 500\text{--}550$ °C), revealing high-sensitivity regions and robust zones. Practically, an optimal configuration recommendation for implementation with energy benefit quantification is provided, identifying trade-offs between power maximization and operational reliability and evaluating potential under future operating conditions. The methodology is applicable to other refineries for aggregate improvement potential identification.

Section 2 presents system description, systematic superstructure development, and mathematical formulation of the optimization problem. Section 3 reports parametric study design and implementation methodology. Section 4 presents identified optimal configurations, parametric space exploration, transition mechanisms, and comparative analysis. Section 6 synthesizes the conclusions and proposes future work.

2. Cogeneration System Description

2.1. Project Context

This work analyzes the cogeneration design for a petroleum refinery in central Mexico. The refinery demands continuous process steam at two pressure levels. An adjacent combined cycle power plant possesses four gas turbines and four heat recovery steam generators that are out of service. The rehabilitation project seeks to integrate both facilities through simultaneous cogeneration of electricity and steam.

This configuration is appropriate for methodological research for three reasons. First, the system presents representative characteristics of industrial cogeneration: multi-pressure process steam requirement (mass flow, pressure, and temperature)s with strict specifications, continuous operation with high reliability, and integration with existing processes. Second, existing equipment has documented specifications that enable methodological validation. Third, a complete redesign allows parametric exploration without limitations of the original configuration.

These characteristics make the system a valuable case study for developing and validating optimization methodologies applicable to other similar projects.

2.2. Gas Turbines

The base generation system consists of four identical gas turbines. Each unit has a nominal capacity of 72 MW. The total installed capacity is 288 MW. The units operated for approximately 35 years before their retirement.

Figure 1 shows a gas turbine train coupled to its HRSG. The system comprises a compressor, a turbine, a combustion chamber, and an electric generator. The gas turbine exhaust gases are utilized in the HRSG to generate steam through three sections: economizer, evaporator, and superheater. In the steam drum, liquid and vapor phases are separated, allowing for the extraction of dry saturated steam for superheating through the superheater.

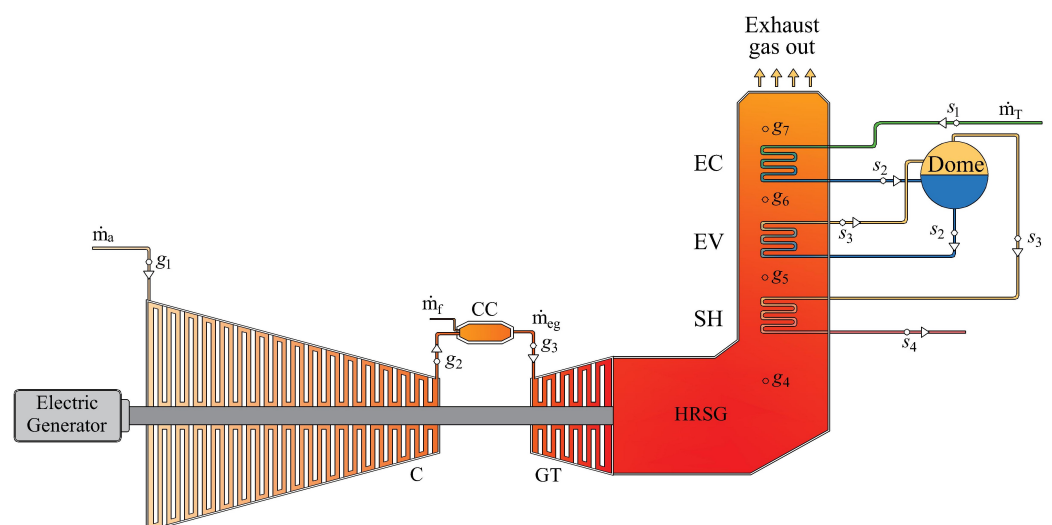


Figure 1. Configuration of a gas turbine unit coupled to its HRSG.

Table 1 presents the operational parameters of the gas turbines. The fuel is natural gas with volumetric composition: 88% CH₄, 10% C₂H₆, 2% C₃H₈. The lower heating value is 49,514 kJ/kg. Combustion gases exit at elevated temperature with significant excess air. These conditions favor steam generation without supplementary firing.

Table 1. Operational parameters of gas turbines.

Parameter	Symbol	Value	Unit
Nominal power per unit	$\dot{W}_{m,TG}$	72	MW
Total electrical power (4 units)	–	288	MW
Turbine inlet temperature	T_{g3}	1250	°C
Compression ratio	π_c	14.0	–
Compressor isentropic efficiency	η_{IC}	0.85	–
Turbine isentropic efficiency	η_{IGT}	0.88	–
Combustor pressure drop	ΔP_{cc}	0.04	–
Turbine outlet pressure drop	ΔP_{GT}	0.04	–

These high-temperature gases feed the HRSGs to generate the steam required by the refinery.

2.3. Process Steam Demands

The refinery requires continuous steam at two pressure levels. Table 2 specifies the design demands. High-pressure (HP) steam represents 11.8% of total demand. This steam feeds units requiring high temperature. Low-pressure (LP) steam represents 88.2% of demand. This steam feeds multiple consumers distributed throughout the refinery.

Table 2. Refinery process steam demands.

Pressure Level	Symbol	Pressure	Temperature	Mass Flow
High pressure (HP)	$\dot{m}_{HP}$	60 bar	482 °C	13.89 kg/s
Low pressure (LP)	$\dot{m}_{LP}$	20 bar	350 °C	104.17 kg/s
Total	–	–	–	118.06 kg/s

This work considers these demands constant at their nominal values. This simplification allows focusing the analysis on steam cycle optimization. Extension to variable demands is identified as future work.

2.4. Heat Recovery Steam Generators

2.4.1. Existing Configuration

Each gas turbine is coupled to a horizontal HRSG with countercurrent flow. The HRSG consists of three main sections, as shown in Figure 1. The economizer preheats feedwater from s_1 to approximately saturation temperature. The evaporator vaporizes water at constant pressure, generating saturated steam in the drum. The superheater heats saturated steam extracted from the drum (s_3) until reaching design temperature (s_4).

Table 3 presents the original design specifications. The HRSGs operated in a single-pressure-level configuration. The total flow from the four units was 163.74 kg/s. This configuration discharged gases to the atmosphere without power cycle integration.

Table 3. Design specifications of existing HRSGs.

Parameter	Symbol	Value	Unit
Steam generation pressure	P_{HRSG}	88.26	bar
Generated steam temperature	T_{s4}	510	°C
Total steam flow (4 units)	$\dot{m}_T$	163.74	kg/s
Pinch point temperature difference	ΔT_{PP}	45	°C
Configuration	–	Single pressure level	

2.4.2. Redesign Scope

The project contemplates a complete HRSG redesign. This design freedom allows systematic parametric exploration. The objective is to identify configurations that maximize electrical generation while satisfying steam demands.

This analysis explores the following parametric ranges. Generation pressure varies between 70 and 140 bar. The lower limit guarantees satisfying HP demand (60 bar) with a margin for pressure drops. The upper limit is determined by metallurgical restrictions at the available gas temperature. Superheating temperature varies between 500 and 560 °C. The lower limit guarantees meeting HP specification (482 °C) with a margin for thermal losses. The upper limit is limited by materials and gas temperature.

This analysis considers a single pressure level configuration to simplify parametric exploration. Extension to multi-pressure configurations is identified as future work. Supplementary firing is not considered. HRSGs utilize only sensible heat from exhaust gases.

For each pressure–temperature combination, steam flow is calculated through a rigorous energy balance. The calculation imposes constraints of minimum pinch point, approach temperature in the superheater, and minimum HRSG stack temperature to avoid acid condensation.

2.5. Reference Conditions

Table 4 presents reference conditions for thermodynamic calculations. Water–steam properties are calculated using IAPWS-IF97 correlations, which are utilized through the XSteam add-in in Excel. Combustion gases are modeled as an ideal gas with constant specific heat $c_p = 1.3428 \text{ kJ}/(\text{kg}\cdot\text{K})$. This value is the weighted average for typical natural gas combustion gas composition with excess air.

Table 4. Reference conditions for thermodynamic analysis.

Parameter	Symbol	Value	Unit
Reference atmospheric pressure	P_0	0.78	bar
Reference ambient temperature	T_0	30	°C
Thermodynamic reference state	–	Saturated liquid water at 30 °C	
Water/steam property model	–	IAPWS-IF97	
Combustion gas model	–	Ideal gas, $c_p = 1.3428 \text{ kJ}/(\text{kg}\cdot\text{K})$	
Condenser temperature difference	ΔT_{COND}	10	°C
Steam turbine isentropic efficiency	η_{IST}	0.89	–
Feedwater pump efficiency	η_{B}	0.85	–

Condenser pressure is calculated as saturation pressure at cooling water temperature plus ΔT_{COND}

$$P_{\text{COND}} = P_{\text{sat}}(T_{\text{amb}} + \Delta T_{\text{COND}}) \quad (1)$$

These conditions are maintained consistently across all calculations presented in this work.

2.6. Proposed System Configuration

Following the repowering performed at the Tula combined cycle power plant, four gas turbines with their respective HRSGs were retired. Additionally, the refinery generates steam independently through conventional boilers. However, this configuration results in relatively low overall efficiency.

The proposed configuration integrates electrical generation with steam supply to the refinery. The system comprises three main elements. First, complete rehabilitation of the four gas turbines and HRSGs to guarantee the supply of steam flows with pressure and temperature parameters demanded by the refinery. Second, installation of an integrated steam cycle including steam turbines with controlled extractions, condenser, pump, makeup tank, and distribution network. Third, a control system for coordinated facility operation.

The proposed system would simultaneously generate electrical power and process steam. Electrical power comes from gas turbines (288 MW) plus the steam cycle. Process steam (13.89 kg/s at 60 bar/482 °C and 104.17 kg/s at 20 bar/350 °C) is extracted from steam turbines.

The central design challenge lies in conflicting objectives. Maximizing electrical power requires expanding all steam to the condenser. Satisfying process demands requires extracting steam at intermediate pressures (60 bar for HP, 20 bar for LP). Extractions reduce the flow available for generation in low-pressure stages. However, extractions are indispensable for refinery specifications. Additionally, steam from the HRSG exceeds the required temperatures. This difference requires reduction strategies without excessive exergy destruction.

The following section presents a systematic formulation of the steam cycle superstructure that resolves these challenges.

3. Steam Cycle Superstructure Formulation

3.1. Optimal Design Problem Statement

The optimal steam cycle design resolves two conflicting objectives. The first objective is to maximize electrical power generation ($\max \dot{W}_{ST}$). The second objective is to satisfy exactly the steam demands ($\dot{m}_{HP} = 13.89$ kg/s at 60 bar/482 °C, $\dot{m}_{LP} = 104.17$ kg/s at 20 bar/350 °C). This multi-objective problem is reformulated as constrained optimization: maximize power subject to exact satisfaction of demands and thermodynamic constraints.

Steam generated in HRSGs must be distributed to three destinations. First, extractions at 60 bar for HP demand. Second, extractions at 20 bar for LP demand. Third, discharge to the condenser of excess flow. The pressure hierarchy must satisfy $P_{HRSG} > P_{HP} > P_{LP} > P_{COND}$. Differences between consecutive levels must allow viable turbine expansion.

Industrial steam turbines require a minimum steam quality in all stages. This constraint avoids mechanical blade erosion from water droplet impact. The established criterion is $x \geq 0.88$ in all expansions, although generally, the last expansion in a steam turbine is where the presence of a two-phase mixture occurs. For saturated or two-phase steam,

$$x = \frac{h - h_f(P)}{h_{fg}(P)} \geq 0.88 \quad (2)$$

where h is specific enthalpy, h_f is saturated liquid enthalpy, and h_{fg} is heat of vaporization at operating pressure. This constraint limits viable expansions and determines which configurations are physically realizable.

3.2. Base Configuration Without Power Utilization

Before introducing steam turbines for additional power generation, the configuration that only satisfies steam demands through expansion valves and tempering mixtures is

analyzed. Figure 2 shows the complete system. The system comprises four distribution headers (Head I, Head II, Head HP, Head LP) and four expansion valves (EV₁–EV₄).

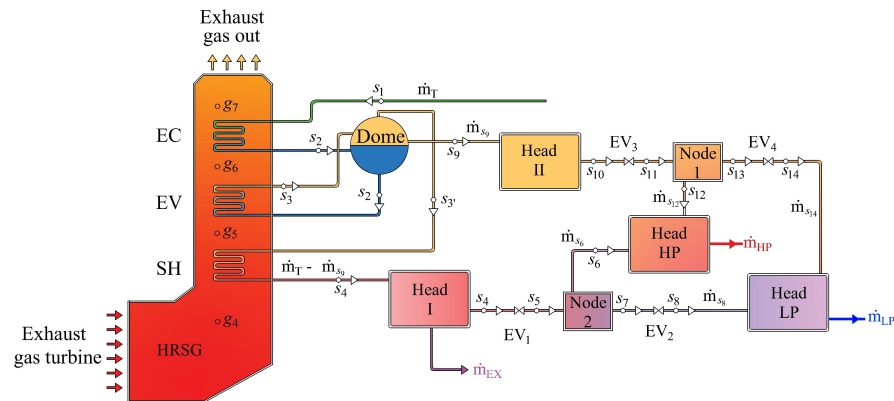


Figure 2. Base configuration with distribution headers and expansion valves.

In this configuration, expansion valves reduce pressure through isenthalpic processes. Head I distributes superheated steam (s_4) from the HRSG. Head II distributes saturated steam (s_3) from the drum. HP and LP headers generate demands through hot and cold stream mixtures. To reach specified temperatures (482 °C for HP, 350 °C for LP), each header requires a specific proportion of hot and cold steam. Excess flow $\dot{m}_{EX}$ is discarded without utilization.

Figure 3 illustrates these processes in temperature–entropy diagram. Vertical lines represent isenthalpic expansions in valves. Red and blue points indicate HP and LP demand conditions, respectively. Superheated steam mixtures with saturated steam allow reaching the required temperatures. The dashed line $x = 0.88$ indicates the quality limit for safe steam turbine operation.

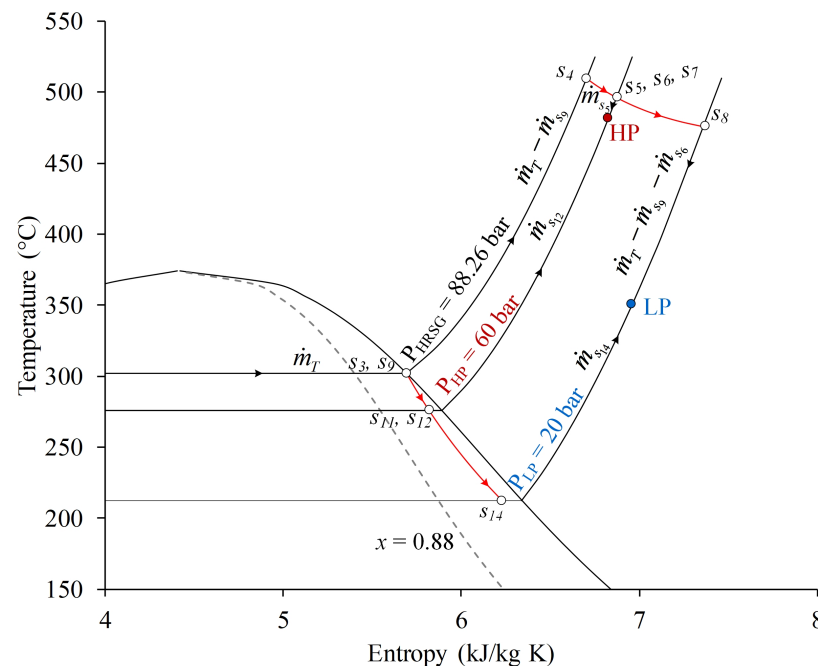


Figure 3. T – s diagram of base configuration showing isenthalpic expansions.

Analysis of processes occurring in expansion valves and headers from the temperature–entropy diagram reveals significant entropy generation. This generation represents an opportunity for power generation. Replacing valves with steam turbines would allow the

utilization of the available pressure differential. This motivation leads to the systematic superstructure derivation presented below.

3.3. Systematic Superstructure Derivation

The steam cycle superstructure is derived through a systematic procedure. This procedure guarantees completeness in viable configuration representation. The method consists of three clearly defined steps. These steps can be applied to any cogeneration system with multi-pressure demands.

3.3.1. Step 1: Pressure Level Definition

Four relevant pressure levels are identified. The HRSG level operates at $P_{\text{HRSG}} = 88.26$ bar (subsequently variable in the range 70–140 bar). The HP level operates at $P_{\text{HP}} = 60$ bar (refinery demand). The LP level operates at $P_{\text{LP}} = 20$ bar (refinery demand). The COND level (excess steam recovery) operates at P_{COND} calculated according to Equation (1).

The number of steam turbines and expansions of each is determined based on superheated steam extractions at the outlet of equipment Head I (s_4), Head HP (HP), EV_1 (s_5), Head LP (LP), EV_2 (s_8); and saturated steam extraction at the outlet of Head II (s_{10}). All extractions can be shown in both Figures 2 and 3.

3.3.2. Step 2: Turbine and Expansion Route Definition

Based on the viable expansions from Step 1, six steam turbines are identified. Each turbine represents a thermodynamically feasible expansion route. Each turbine is characterized by its route (sequence of pressure levels), number of stages, and available extraction points.

An expansion stage is a continuous segment between two consecutive levels without intermediate extractions. The number of stages corresponds to the number of segments in the route. Extractions for demands occur between stages, at intermediate pressure levels.

Table 5 presents the six systematically defined turbines. ST_1 and ST_2 have three stages and allow extractions at HP and LP pressures. ST_3 starts at HP Header, has two stages, and allows extraction at LP pressure. ST_4 has two stages and allows extraction at LP pressure. ST_5 has one stage and no extractions. ST_6 starts at LP Header and has no extractions.

Table 5. Systematic definition of steam turbines in the superstructure.

State	Turbine	Expansion Route	Stages	Extractions
(s_4)	ST_1	HRSG $\rightarrow$ HP $\rightarrow$ LP $\rightarrow$ COND	3	HP, LP
(s_{10})	ST_2	HRSG $\rightarrow$ HP $\rightarrow$ LP $\rightarrow$ COND	3	HP, LP
(HP)	ST_3	HP $\rightarrow$ LP $\rightarrow$ COND	2	LP
(s_5)	ST_4	HP $\rightarrow$ LP $\rightarrow$ COND	2	LP
(s_8)	ST_5	LP $\rightarrow$ COND	1	None
(LP)	ST_6	LP $\rightarrow$ COND	1	None

The three evaluated configurations are the systematic outcome of this procedure, not an arbitrary selection. ST_2 is excluded because its inlet state s_{10} (saturated drum steam) produces steam quality below 0.88 in the final expansion stage across the entire parametric range, violating Equation (31). ST_6 duplicates the LP $\rightarrow$ COND expansion route of ST_5 without additional routing flexibility, yielding identical or lower net power in all evaluated cases.

This definition guarantees three important properties. First, each stage corresponds to a physical turbine segment with continuous flow. Second, the number of stages reflects the geometric complexity of the turbine. Third, extractions between stages allow independent flow control to match any necessary demands.

3.3.3. Step 3: Integration of Expansions in T - s Diagram

According to the location and number of expansions of the six steam turbines, the number of streams entering and leaving HP and LP headers can now be identified. In this way, Figure 4 illustrates the complete superstructure in the temperature–entropy diagram. The diagram shows the multiple possible expansion routes from the HRSG level (s_4) to the condenser. Routes include direct expansions (ST_4 , ST_5) and expansions with extractions at HP or LP (ST_1 , ST_2 , ST_3 , and ST_6). The left side shows expansions from drum saturated steam (s_3).

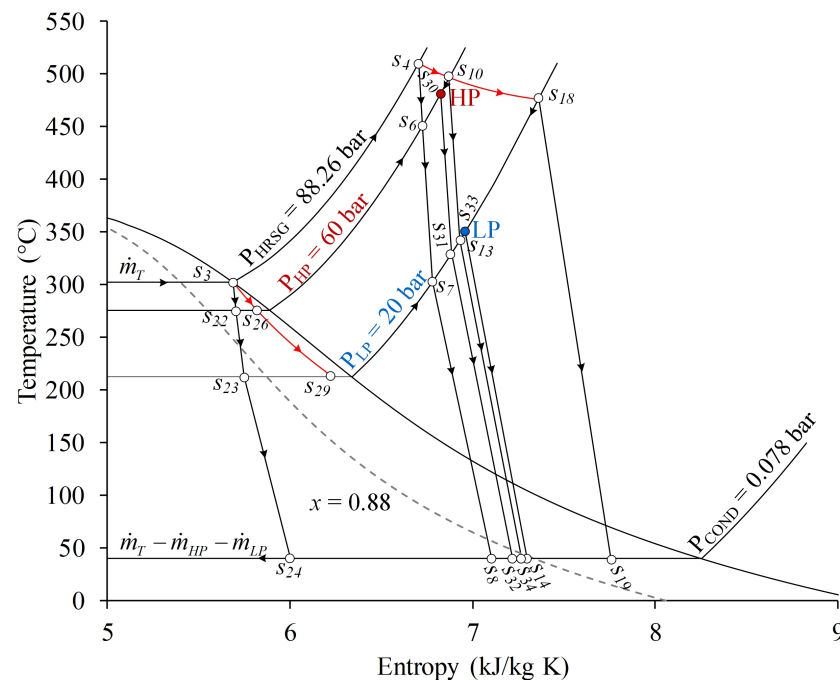


Figure 4. T - s diagram of superstructure showing multiple expansion routes.

The dashed line $x = 0.88$ delimits the safe operation region for steam turbines. Red streams represent HP steam at 60 bar and 482 °C. Blue streams represent LP steam at 20 bar and 350 °C.

The multiple routes illustrated from the T - s diagram represent a theoretical approach that, in turn, can be put into practice. This allows the algorithm to select the optimal combination. Selection maximizes power generation, satisfying all thermodynamic and demand constraints.

3.4. Complete Superstructure Visualization

The six defined turbines integrate with headers, demands, condenser, and feedwater system. Figure 5 shows the complete superstructure. The system integrates the six turbines with different routes according to Table 5. Distribution headers allow stream mixing. Valves EV_1 – EV_4 provide alternative routes without power generation. Bifurcation nodes (Node 1–3) distribute flows between multiple destinations. The condenser operates at pressure calculated according to Equation (1). Makeup tank and pump close the cycle.

Lines with valves represent optional streams. Binary variables activate or deactivate these streams in optimization. Optimal configuration is determined by selecting the turbine and stream subset that maximizes $\dot{W}_{ST}$. Selection must satisfy steam quality and exact process demand constraints.

The superstructure contains binary variables to activate/deactivate stages and streams. It also contains continuous variables for mass flows and powers. Optimal configurations

are identified through MINLP optimization. The objective is to maximize total steam cycle power. Constraints include mass and energy balances, steam quality as specified by Equation (2), and exact demand satisfaction.

The presented methodology is systematic and generalizable. To apply it to another cogeneration system requires three steps. First, identify pressure levels according to specific demands. Second, define turbines corresponding to viable routes, specifying stages and extraction points. Third, integrate all elements into a superstructure with explicit binary variables. The resulting problem has a standard MINLP structure solvable with commercial solvers.

The following section presents a detailed mathematical model of the superstructure, including balance equations, thermodynamic constraints, and the formulation of an optimization problem.

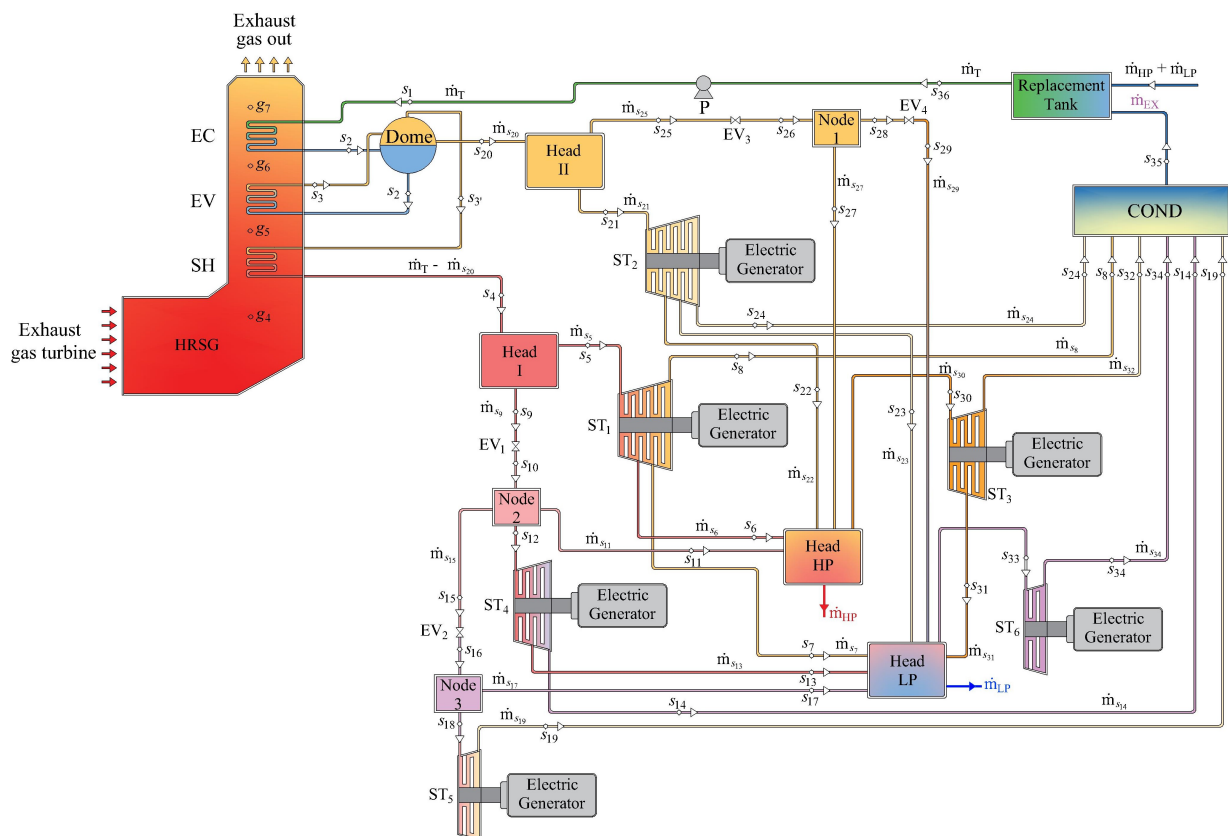


Figure 5. Complete steam cycle superstructure with six alternative turbines.

4. Mathematical Modeling and Optimization

4.1. Assumptions and Considerations

Thermodynamic modeling is developed under the assumptions presented below, complementing reference conditions and equipment parameters established in Section 2.

4.1.1. Operational Assumptions

- Steady state: all components operate at nominal design conditions. This assumption is appropriate for configuration optimization where the interest is in design point performance.
- Adiabatic operation: heat losses to the environment are neglected in all components.
- Identical unit operation: The four gas turbines and HRSGs operate under identical conditions.

4.1.2. Thermodynamic Assumptions

- Perfect gas model for Brayton cycle: combustion air and gases in the gas turbine are modeled as ideal gases with constant specific heats and isentropic exponents. For air in compressor: $c_{p,a} = 1.005 \text{ kJ}/(\text{kg}\cdot\text{K})$, $\gamma_a = 1.4$. For combustion gases in turbine: $c_{p,eg} = 1.3428 \text{ kJ}/(\text{kg}\cdot\text{K})$, $\gamma_{eg} = 1.2972$. Isentropic exponents are calculated as $x_a = (\gamma_a - 1)/\gamma_a = 0.286$ and $x_{eg} = (\gamma_{eg} - 1)/\gamma_{eg} = 0.218$ for pressure and temperature expressions presented in the following subsection.
- Complete combustion in the chamber is considered complete with 161.90% excess air. Fuel-air ratio (far) is determined through energy balance in the combustion chamber. Unburned emissions are neglected, given excess air and high combustion temperatures.
- Pressure drops in gas turbine (ΔP_{CC} , ΔP_{GT}) are explicitly considered according to Table 1.
- Pressure drops in pipes, headers, and superstructure equipment are neglected.

4.2. Thermodynamic Modeling of Components

Models are developed consistently with Section 4.1 assumptions and Section 2 parameters. Water and steam properties are evaluated using IAPWS-IF97 correlations, which are utilized through the XSteam add-in in Excel.

4.2.1. Gas Turbine Cycle

The Brayton cycle of each turbine is characterized by thermodynamic states presented in Table 6. Isentropic exponents are $x_a = 0.286$ for air and $x_{eg} = 0.218$ for combustion gases.

Table 6. Thermodynamic states of gas turbine cycle.

State	Pressure	Temperature
g_1	P_{atm}	T_{amb}
g_2	$P_{g_1} \pi_C$	$T_{g_1} \left[1 + \frac{1}{\eta_{IC}} (\pi_C^{x_a} - 1) \right]$
g_3	$P_{g_2} (1 - \Delta P_{CC})$	T_{g_3}
g_4	$P_{g_1} (1 + \Delta P_{GT})$	$T_{g_3} \left\langle 1 - \eta_{IGT} \left\{ 1 - \frac{(1 + \Delta P_{GT})^{x_{eg}}}{[\pi_C (1 - \Delta P_{CC})]^{x_{eg}}} \right\} \right\rangle$

The total air flow processed by N gas turbines is

$$\dot{m}_a = \frac{\dot{W}_{m,GT}}{c_{p,a} T_{g_1} \left\{ (1 + far) \frac{c_{p,eg}}{c_{p,a}} \eta_{IGT} \left[1 - \frac{(1 + \Delta P_{GT})^{x_{eg}}}{[\pi_C (1 - \Delta P_{CC})]^{x_{eg}}} \right] - \frac{1}{\eta_{IC}} (\pi_C^{x_a} - 1) \right\}} \quad (3)$$

The fuel–air ratio is derived from the adiabatic combustion chamber energy balance (complete combustion): $\dot{m}_a c_{p,a} T_{g_2} + \dot{m}_f LHV = (\dot{m}_a + \dot{m}_f) c_{p,eg} T_{g_3}$. Dividing by $\dot{m}_a$ and solving for $far = \dot{m}_f / \dot{m}_a$ yields Equation (5) directly.

For the case study, $N = 4$ turbines and $\dot{W}_{m,GT} = 288 \text{ MW}$. Fuel-air ratio is obtained from the combustor balance

$$far = \frac{c_{p,eg} T_{g_3} - c_{p,a} T_{g_2}}{LHV - c_{p,eg} T_{g_3}} \quad (4)$$

The total heat supplied in N chambers is

$$\dot{Q}_{\text{sup,CC}} = \dot{m}_a c_{p,a} T_{g_1} \left[(1 + far) \frac{c_{p,eg}}{c_{p,a}} \frac{T_{g_3}}{T_{g_1}} - 1 - \left(\frac{\pi_C^{x_a} - 1}{\eta_{IC}} \right) \right] \quad (5)$$

The total fuel and exhaust gas flows are

$$\dot{m}_f = \frac{\dot{Q}_{\text{sup,CC}}}{LHV}, \quad \dot{m}_{eg} = \dot{m}_a + \dot{m}_f \quad (6)$$

4.2.2. Heat Recovery Steam Generator

HRSG modeling is performed for one unit and scaled by N . Generated steam flow is determined through energy balance with pinch point constraint:

$$\dot{m}_T = \frac{\dot{m}_{eg} c_{p,eg} (T_{g4} - T_{g6})}{h_4 - h_2}, \quad \Delta T_{PP} = T_{g6} - T_{\text{sat}}(P_{\text{HRSG}}) \quad (7)$$

Substituting pinch point constraint ($\Delta T_{PP} = 10^\circ\text{C}$):

$$\dot{m}_T = \frac{\dot{m}_{eg} c_{p,eg} [T_{g4} - (T_{\text{sat}}(P_{\text{HRSG}}) + 10)]}{h_4 - h_2} \quad (8)$$

Gas temperatures at the superheater and economizer outlet are

$$T_{g5} = T_{g4} - \frac{\dot{m}_T (h_4 - h_3)}{\dot{m}_{eg} c_{p,eg}}, \quad T_{g7} = T_{g6} - \frac{\dot{m}_T (h_2 - h_1)}{\dot{m}_{eg} c_{p,eg}} \quad (9)$$

Stack temperature must satisfy $T_{g7} \geq 120^\circ\text{C}$.

4.2.3. Balances in Superstructure Components

The superstructure integrates 21 main components whose mass and energy balances are presented in Table 7. Thermodynamic states are identified by numerical subscripts (h_i , $\dot{m}_i$ where $i = 1, 2, \dots, 36$) according to Figure 5.

The fundamental thermodynamic equations governing table processes are the following. For steam turbine expansions,

$$s_{\text{out,s}} = s_{\text{in}}, \quad h_{\text{out}} = h_{\text{in}} - \eta_{\text{is}}(h_{\text{in}} - h_{\text{out,s}}), \quad \dot{W} = \dot{m}_{\text{in}}(h_{\text{in}} - h_{\text{out}}) \quad (10)$$

where $h_{\text{out,s}} = h(P_{\text{out}}, s_{\text{out,s}})$. For adiabatic mixing in headers,

$$h_{\text{mix}} = \frac{\sum_i \dot{m}_i h_i}{\sum_i \dot{m}_i} \quad (11)$$

For isenthalpic expansions in valves,

$$h_{\text{out}} = h_{\text{in}} \quad (12)$$

For bifurcations at nodes and at Headers I and II,

$$\dot{m}_{\text{in}} = \sum_j \dot{m}_{\text{out},j}, \quad h_{\text{out},j} = h_{\text{in}} \quad \forall j \quad (13)$$

Steam quality is calculated using

$$x = \frac{h - h_f(P)}{h_{fg}(P)} \quad (14)$$

Condensing pressure and pumping work are determined by

$$P_{\text{COND}} = P_{\text{sat}}(T_{\text{amb}} + \Delta T_{\text{COND}}), \quad \dot{W}_P = \frac{\dot{m}_T (P_{\text{HRSG}} - P_{\text{COND}}) v_{\text{liq}}}{\eta_{\text{pump}}} \quad (15)$$

The presented models constitute the basis for the optimization problem formulation presented in the following subsection.

Table 7. Superstructure steam cycle components with mass and energy balances.

Comp.	States	Mass Balance	Energy Balance	Process/Notes
HRSG System				
EC	1 → 2	$\dot{m}_1 = \dot{m}_2 = \dot{m}_T$	$\dot{m}_{eg} c_{p, eg} (T_{g7} - T_{g6}) = \dot{m}_T (h_2 - h_1)$	Isobaric, P_{HRSG} , preheating
EV	2 → 3	$\dot{m}_2 = \dot{m}_3$	Equation (8)	Isobaric-isothermal, P_{HRSG} , T_{sat} , $\Delta T_{PP} = 10$ °C
SH	3 → 4	$\dot{m}_3 = \dot{m}_4 = \dot{m}_T - \dot{m}_{20}$	$\dot{m}_{eg} c_{p, eg} (T_{g4} - T_{g3}) = (\dot{m}_T - \dot{m}_{20}) (h_4 - h_3)$	Isobaric, P_{HRSG} , SH steam at T_{s4}
Drum	2, 3 → 2', 3', 20	$\dot{m}_3 = \dot{m}_{3'} + \dot{m}_{20}$	L-V Sep: 3 (sat), 4 (SH)	Isobaric-isothermal, P_{HRSG} , T_{sat}
Distribution Network				
Head I	4 → 5, 9	$\dot{m}_4 = \dot{m}_5 + \dot{m}_9$	$h_5 = h_9 = h_4$	Isobaric, P_{HRSG} , bifurcation
Head II	20 → 21, 25	$\dot{m}_{20} = \dot{m}_{21} + \dot{m}_{25}$	$h_{21} = h_{25} = h_{20}$	Isobaric, P_{HRSG} , bifurcation
Head HP	6, 11, 22, 27 → 30, HP	$\dot{m}_6 + \dot{m}_{11} + \dot{m}_{22} + \dot{m}_{27} = \dot{m}_{30} + \dot{m}_{HP}$	$\sum \dot{m}_i h_i = \dot{m}_{30} h_{30} + \dot{m}_{HP} h_{HP}$	Isobaric, $P_{HP} = 60$ bar, $T_{HP} = 482$ °C
Head LP	7, 13, 17, 23, 29, 31 → 33, LP	$\dot{m}_7 + \dot{m}_{13} + \dot{m}_{17} + \dot{m}_{23} + \dot{m}_{29} + \dot{m}_{31} = \dot{m}_{33} + \dot{m}_{LP}$	$\sum \dot{m}_i h_i = \dot{m}_{33} h_{33} + \dot{m}_{LP} h_{LP}$	Isobaric, $P_{LP} = 20$ bar, $T_{LP} = 350$ °C
Expansion Valves				
EV ₁	9 → 10	$\dot{m}_9 = \dot{m}_{10}$	$h_{10} = h_9$	Isenthalpic, $P_{HRSG} \rightarrow P_{HP}$
EV ₂	15 → 16	$\dot{m}_{15} = \dot{m}_{16}$	$h_{16} = h_{15}$	Isenthalpic, $P_{HP} \rightarrow P_{LP}$
EV ₃	25 → 26	$\dot{m}_{25} = \dot{m}_{26}$	$h_{26} = h_{25}$	Isenthalpic, $P_{HRSG} \rightarrow P_{HP}$
EV ₄	28 → 29	$\dot{m}_{28} = \dot{m}_{29}$	$h_{29} = h_{28}$	Isenthalpic, $P_{HP} \rightarrow P_{LP}$
Bifurcation Nodes				
Node 1	26 → 27, 28	$\dot{m}_{26} = \dot{m}_{27} + \dot{m}_{28}$	$h_{27} = h_{28} = h_{26}$	Isobaric, P_{HP} , bifurcation
Node 2	10 → 11, 12, 15	$\dot{m}_{10} = \dot{m}_{11} + \dot{m}_{12} + \dot{m}_{15}$	$h_{11} = h_{12} = h_{15} = h_{10}$	Isobaric, P_{HP} , bifurcation
Node 3	16 → 17, 18	$\dot{m}_{16} = \dot{m}_{17} + \dot{m}_{18}$	$h_{17} = h_{18} = h_{16}$	Isobaric, P_{LP} , bifurcation
Steam Turbines				
ST ₁	5 → 6, 7, 8	$\dot{m}_5 = \dot{m}_6 + \dot{m}_7 + \dot{m}_8$	$\dot{m}_5 h_5 = \dot{m}_6 h_6 + \dot{m}_7 h_7 + \dot{m}_8 h_8 + \dot{W}_{ST_1}$	3 stages: $P_{HRSG} \rightarrow P_{HP} \rightarrow P_{LP} \rightarrow P_{COND}$, $x_i \geq 0.88$
ST ₂	21 → 22, 23, 24	$\dot{m}_{21} = \dot{m}_{22} + \dot{m}_{23} + \dot{m}_{24}$	$\dot{m}_{21} h_{21} = \dot{m}_{22} h_{22} + \dot{m}_{23} h_{23} + \dot{m}_{24} h_{24} + \dot{W}_{ST_2}$	3 stages: $P_{HRSG} \rightarrow P_{HP} \rightarrow P_{LP} \rightarrow P_{COND}$, $x_i \geq 0.88$
ST ₃	30 → 31, 32	$\dot{m}_{30} = \dot{m}_{31} + \dot{m}_{32}$	$\dot{m}_{30} h_{30} = \dot{m}_{31} h_{31} + \dot{m}_{32} h_{32} + \dot{W}_{ST_3}$	2 stages: $P_{HP} \rightarrow P_{LP} \rightarrow P_{COND}$, $x_i \geq 0.88$
ST ₄	12 → 13, 14	$\dot{m}_{12} = \dot{m}_{13} + \dot{m}_{14}$	$\dot{m}_{12} h_{12} = \dot{m}_{13} h_{13} + \dot{m}_{14} h_{14} + \dot{W}_{ST_4}$	2 stages: $P_{HP} \rightarrow P_{LP} \rightarrow P_{COND}$, $x_i \geq 0.88$
ST ₅	18 → 19	$\dot{m}_{18} = \dot{m}_{19}$	$\dot{m}_{18} h_{18} = \dot{m}_{19} h_{19} + \dot{W}_{ST_5}$	1 stage: $P_{LP} \rightarrow P_{COND}$, $x_{19} \geq 0.88$
ST ₆	33 → 34	$\dot{m}_{33} = \dot{m}_{34}$	$\dot{m}_{33} h_{33} = \dot{m}_{34} h_{34} + \dot{W}_{ST_6}$	1 stage: $P_{LP} \rightarrow P_{COND}$, $x_{34} \geq 0.88$
Condensate System				
COND	8, 14, 19, 24, 32, 34 → 35	$\sum \dot{m}_{i, in} = \dot{m}_{35}$	$\sum \dot{m}_i h_i = \dot{m}_{35} h_{35} + \dot{Q}_{COND}$	Isobaric-isothermal, P_{COND} , T_{sat} , Equation (1)
RT	IN, 35 → 36	$\dot{m}_{HP} + \dot{m}_{LP} + \dot{m}_{35} = \dot{m}_T$	$(\dot{m}_{HP} + \dot{m}_{LP}) h_{IN} + \dot{m}_{35} h_{35} = \dot{m}_T h_{36}$	Isobaric, P_{COND} , water makeup
Pump	36 → 1	$\dot{m}_{36} = \dot{m}_1 = \dot{m}_T$	$\dot{m}_{36} h_{36} + \dot{W}_P = \dot{m}_1 h_1$	Approx. isothermal, $P_{COND} \rightarrow P_{HRSG}$, Equation (1)

4.3. Optimization Problem Formulation and Configuration Enumeration Approach

The optimization problem is formulated as a mixed-integer nonlinear program (MINLP) to determine the optimal steam cycle configuration that maximizes electrical power generation while simultaneously satisfying refinery steam demands. The formulation integrates Section 4.2 thermodynamic models with discrete decision variables for equipment and stream activation.

4.3.1. Decision Variables

The problem contains two variable types that completely characterize system state.

Continuous Variables

Continuous variables ($n_c = 43$) describe mass flows and thermodynamic properties of all superstructure streams:

- Mass flows: $\dot{m}_i$ for $i = 1, 2, \dots, 36$ according to Table 7.
- Specific enthalpies: h_i determined by pressure, temperature and phase through IAPWS-IF97 correlations.
- Derived properties: temperature T_i , quality x_i (calculated, not independent).
- Generated powers: $\dot{W}_{ST_j}$ for $j = 1, \dots, 6$ according to Equation (20).
- Pumping work: $\dot{W}_P$ according to Equation (21).

Binary Variables

Binary variables ($n_b = 24$) control turbine stage and flow stream activation:

$$y_{j,k} = \begin{cases} 1 & \text{if stage } k \text{ of turbine } j \text{ is active} \\ 0 & \text{otherwise} \end{cases} \quad (16)$$

where $j \in \{1, 2, 3, 4, 5, 6\}$ and k varies according to each turbine's number of stages: ST₁ and ST₂ (3 stages), ST₃ and ST₄ (2 stages), ST₅ and ST₆ (1 stage). Total number of turbine binary variables is 12.

Additionally, 12 binary variables control stream existence in superstructure alternative routes (valves EV₁–EV₄ and node bifurcations).

4.3.2. Objective Function

The objective function maximizes net power generated by the steam cycle is

$$\max \quad \dot{W}_{\text{net}} = \sum_{j=1}^6 \dot{W}_{\text{ST}_j} - \dot{W}_P \quad (17)$$

Power generated by each turbine $\dot{W}_{\text{ST}_j}$ is calculated through expansion with isentropic efficiency. For each expansion stage, the isentropic outlet state is determined by

$$s_{\text{out},s} = s_{\text{in}}, \quad h_{\text{out},s} = h(P_{\text{out}}, s_{\text{out},s}) \quad (18)$$

Actual outlet enthalpy is obtained applying isentropic efficiency ($\eta_{\text{is}} = 0.89$):

$$h_{\text{out}} = h_{\text{in}} - \eta_{\text{is}}(h_{\text{in}} - h_{\text{out},s}) \quad (19)$$

Power generated by each turbine stage is

$$\dot{W}_{\text{ST}_j} = \dot{m}_{\text{in}}(h_{\text{in}} - h_{\text{out}}) \quad (20)$$

These equations apply to each of the 12 expansion stages of the six turbines according to Table 7 configuration. For multi-stage turbines (ST₁–ST₄), total power is the sum of all active stage powers.

Pumping work is calculated using

$$\dot{W}_P = \frac{\dot{m}_T(P_{\text{HRSG}} - P_{\text{COND}})v_{\text{liq}}}{\eta_{\text{pump}}} \quad (21)$$

where $v_{\text{liq}} = 0.001 \text{ m}^3/\text{kg}$ is liquid water specific volume and $\eta_{\text{pump}} = 0.85$ according to Table 4. Although $\dot{W}_P$ typically represents 0.5–1% of turbine-generated power, it is included for rigorous energy accounting. Condensing pressure P_{COND} is determined according to Equation (1).

4.3.3. Constraints

Problem constraints are classified into five categories that guarantee physical, thermodynamic and operational solution feasibility.

Mass Balance Constraints

The 21 mass balances from Table 7 must be simultaneously satisfied:

$$\sum_{i \in \text{IN}_c} \dot{m}_i = \sum_{j \in \text{OUT}_c} \dot{m}_j \quad \forall c \in C \quad (22)$$

where $\mathcal{C}$ is the set of 21 components, IN_c and OUT_c denote component c input and output streams. These balances include HRSG (economizer, evaporator, superheater, drum), distribution network (four headers, three nodes), expansion valves (EV_1 – EV_4), turbines (ST_1 – ST_6), and condensate system (condenser, tank, pump).

Energy Balance Constraints

The 11 energy balances for components with conversion or mixing from Table 7 are imposed as equality constraints. For turbines:

$$\dot{m}_{\text{in},j} h_{\text{in},j} = \sum_k \dot{m}_{\text{out},j,k} h_{\text{out},j,k} + \dot{W}_{\text{ST}_j} \quad \forall j \in \{1, \dots, 6\} \quad (23)$$

where outlet enthalpies $h_{\text{out},j,k}$ are calculated according to Equations (18) and (19) and powers $\dot{W}_{\text{ST}_j}$ according to Equation (20).

For mixing headers (Head HP, Head LP):

$$\sum_{i \in \text{IN}_h} \dot{m}_i h_i = \sum_{j \in \text{OUT}_h} \dot{m}_j h_j \quad \forall h \in \{\text{HP}, \text{LP}\} \quad (24)$$

These balances guarantee that Head HP and Head LP mixtures generate steam at specified temperatures ($T_{\text{HP}} = 482^\circ\text{C}$, $T_{\text{LP}} = 350^\circ\text{C}$).

Refinery Demand Constraints

High- and low-pressure steam demands are satisfied exactly:

$$\dot{m}_{\text{HP}} = 13.89 \text{ kg/s}, \quad \dot{m}_{\text{LP}} = 104.17 \text{ kg/s} \quad (25)$$

with temperature specifications $T_{\text{HP}} = 482^\circ\text{C}$ and $T_{\text{LP}} = 350^\circ\text{C}$ according to Table 7. These constraints are inviolable and represent refinery operational requirements.

Thermodynamic Constraints

Steam quality at each turbine stage outlet is calculated using

$$x_{j,k} = \frac{h_{j,k} - h_f(P_{j,k})}{h_{fg}(P_{j,k})} \quad (26)$$

where $h_f(P_{j,k})$ is saturated liquid enthalpy and $h_{fg}(P_{j,k})$ is heat of vaporization at pressure $P_{j,k}$ of stage k of turbine j . Minimum quality constraint is imposed on all stages:

$$x_{j,k} \geq 0.88 \quad \forall j \in \{1, \dots, 6\}, \quad \forall k \quad (27)$$

This constraint is critical to prevent turbine blade erosion caused by high-velocity liquid water droplet impact. The constraint only applies when expansion results in wet steam (two-phase region). For superheated steam, the constraint is automatically satisfied.

This thermodynamic constraint is particularly important because it causes discrete transitions between optimal configurations when certain expansion routes violate the quality limit. Specifically, for low steam generation pressures ($P_{\text{HRSG}} < 80$ bar) and high superheater outlet temperature T_{s4s} ($T_{s4s} > 530^\circ\text{C}$), complete expansions of ST_1 and ST_2 from P_{HRSG} to P_{COND} result in qualities below 0.88, forcing the optimizer to use alternative routes with expansion valves.

Gas temperature at economizer outlet (stack) must satisfy

$$T_{g7} \geq 120^\circ\text{C} \quad (28)$$

According to Equation (9), to avoid water vapor condensation and acid formation in the stack.

Activation Logic Constraints

Logic constraints couple binary variables with mass flows through the big-M formulation:

$$\dot{m}_{j,k} \leq y_{j,k} \cdot M_{j,k} \quad \forall j, k \quad (29)$$

where $M_{j,k}$ is a sufficiently large upper bound for flow in stage k of turbine j . In this work, $M_{j,k} = 150$ kg/s is used (approximately total generated steam flow). When $y_{j,k} = 0$, $\dot{m}_{j,k} = 0$ is forced (inactive stage). When $y_{j,k} = 1$, flow can take any value between 0 and $M_{j,k}$.

Additionally, hierarchical precedence between stages of the same turbine is imposed:

$$y_{j,k+1} \leq y_{j,k} \quad \forall j, \quad k = 1, \dots, n_j - 1 \quad (30)$$

where n_j is the number of stages of turbine j . This constraint guarantees that a later stage cannot be activated if the previous stage is inactive. For example, for ST₁ with three stages: if $y_{1,1} = 0$ then $y_{1,2} = y_{1,3} = 0$ obligatorily.

Steam quality constraint violation (Equation (27)) forces the corresponding binary variable to zero:

$$x_{j,k} < 0.88 \implies y_{j,k} = 0 \quad (31)$$

This formulation allows the optimizer to automatically exclude configurations that would violate thermodynamic limits. In practice, this constraint is implemented through an explicit pre-feasibility filter: before invoking the NLP solver, the isentropic outlet enthalpy of each stage is evaluated. If $h_{j,k} - h_f(P_{j,k}) < 0.88 h_{fg}(P_{j,k})$ for any stage, the configuration is excluded without NLP evaluation.

4.3.4. Complete MINLP Problem Formulation

The complete problem is expressed as

$$\begin{aligned} \max_{\dot{m}_i, h_i, y_{j,k}} \quad & \dot{W}_{\text{net}} = \sum_{j=1}^6 \dot{W}_{\text{ST}_j} - \dot{W}_P \\ \text{s.t.} \quad & \text{Mass balances (21 constraints): Equation (22)} \\ & \text{Energy balances (11 constraints): Equations (23) and (24)} \\ & \text{Refinery demands (2 constraints): Equation (25)} \\ & \text{Steam quality (12 constraints): Equation (27)} \\ & \text{Stack temperature (1 constraint): Equation (28)} \\ & \text{Big-M activation (12 constraints): Equation (29)} \\ & \text{Stage precedence (8 constraints): Equation (30)} \\ & \text{Thermodynamic properties: Equations (18)–(21)} \\ & \dot{m}_i \geq 0 \quad \forall i \\ & y_{j,k} \in \{0, 1\} \quad \forall j, k \end{aligned} \quad (32)$$

The problem contains 67 variables (43 continuous + 24 binary) and approximately 67 constraints.

4.3.5. Computational Implementation

The MINLP optimization problem formulated in Sections 4.3.1–4.3.3 was implemented in Microsoft Excel 2019 with GRG (Generalized Reduced Gradient) Nonlinear solver and XSteam add-in version 2.6 for thermodynamic properties evaluation based on IAPWS-IF97 correlations. The solver was configured with convergence tolerance 10^{-6} , constraint preci-

sion 10^{-5} , and configuration enumeration approach evaluating three topologically distinct candidate configurations at each parametric point, with multistart strategy (10 runs) for continuous variable optimization to address the non-convex nature of the problem arising from thermodynamic nonlinearities and bilinear terms. The complete solver configuration is provided in Table 8.

Table 8. GRG Nonlinear Solver Configuration (per NLP subproblem).

Parameter	Value	Purpose
Convergence tolerance	10^{-6}	Gradient norm threshold
Constraint precision	10^{-5}	Feasibility tolerance
Maximum iterations	1000	Prevents infinite loops
Multistart runs	10	Continuous variable initialization
Population size	50	Random perturbation magnitude
Number of candidate configs	3	Configuration enumeration

The solution algorithm follows a five-step procedure for each parametric case (P_{HRSG}, T_{s4}): (1) calculate HRSG steam generation $\dot{m}T$ from gas turbine exhaust conditions using energy balance with pinch point constraint (Equation (8)), (2) identify three candidate configurations based on thermodynamic viability (Configuration 1: $ST_1 + ST_3 + ST_5$; Configuration 2: $ST_1 + ST_4 + ST_5$; Configuration 3: $ST_1 + ST_3 + ST_4$), (3) for each candidate configuration, solve NLP with binary variables fixed, using multistart strategy for continuous variable optimization, (4) select configuration generating maximum power among feasible candidates, and (5) validate solution through three-level protocol verifying thermodynamic consistency (energy/mass balance closure $< 0.1\%$), physical feasibility (steam quality $x_{jk} \geq 0.88$, pressure hierarchy), and solution quality (convergence achieved, multistart consistency within 0.1%). Typical solution time is 2–5 min per case on standard hardware (Intel Core i7-9700, 16 GB RAM).

The parametric analysis systematically evaluates 84–105 operating points combining pressure sweep $P_{\text{HRSG}} = [70, 75, 88.26, 90, 100, 110, 120, 130, 140]$ bar with temperature ranges $T_{s4} = [500, 510, 520]$ °C (low range, 27 cases), $[530, 540]$ °C (mid range, 18 cases), and $[550, 560]$ °C (high range, 18 cases), plus nominal case (88.26 bar, 510 °C) and additional validation points. Independent configuration evaluation is performed at each parametric combination (three NLP subproblems per point), with 98.7% of cases (83/84) passing all validation checks on first attempt. Total computational time for complete parametric map is 7–9 h on the specified hardware, reducible through parallel execution across multiple processor cores.

Solver Limitations and Optimality Claims

The configuration enumeration approach employed provides locally optimal solutions within each of the three candidate topologies systematically evaluated but does not guarantee global optimality across all 2^{24} possible binary variable combinations. Throughout this manuscript, “optimal” refers to locally optimal solutions among the three candidates, not to proven global optimality. This approach balances computational tractability with thermodynamic rigor, as evidenced by coherent regional patterns in Table 10 and mechanistically consistent thermodynamic explanations in Section 5.3.

Complete computational details including algorithm pseudocode, detailed validation protocol specifications, input data (natural gas composition, reference environment conditions), and data availability statement are provided in Appendix B to ensure full reproducibility of results.

Figure 6 presents the flowchart of the entire proposed methodology for the optimization of the cogeneration system superstructure. It synthesizes the systematic five-step procedure, integrating everything from the superstructure definition and the MINLP model to the validation of results and the generation of the optimal configuration map. This visual scheme consolidates the comprehensive approach developed to address the simultaneous optimization of parameters and topology.

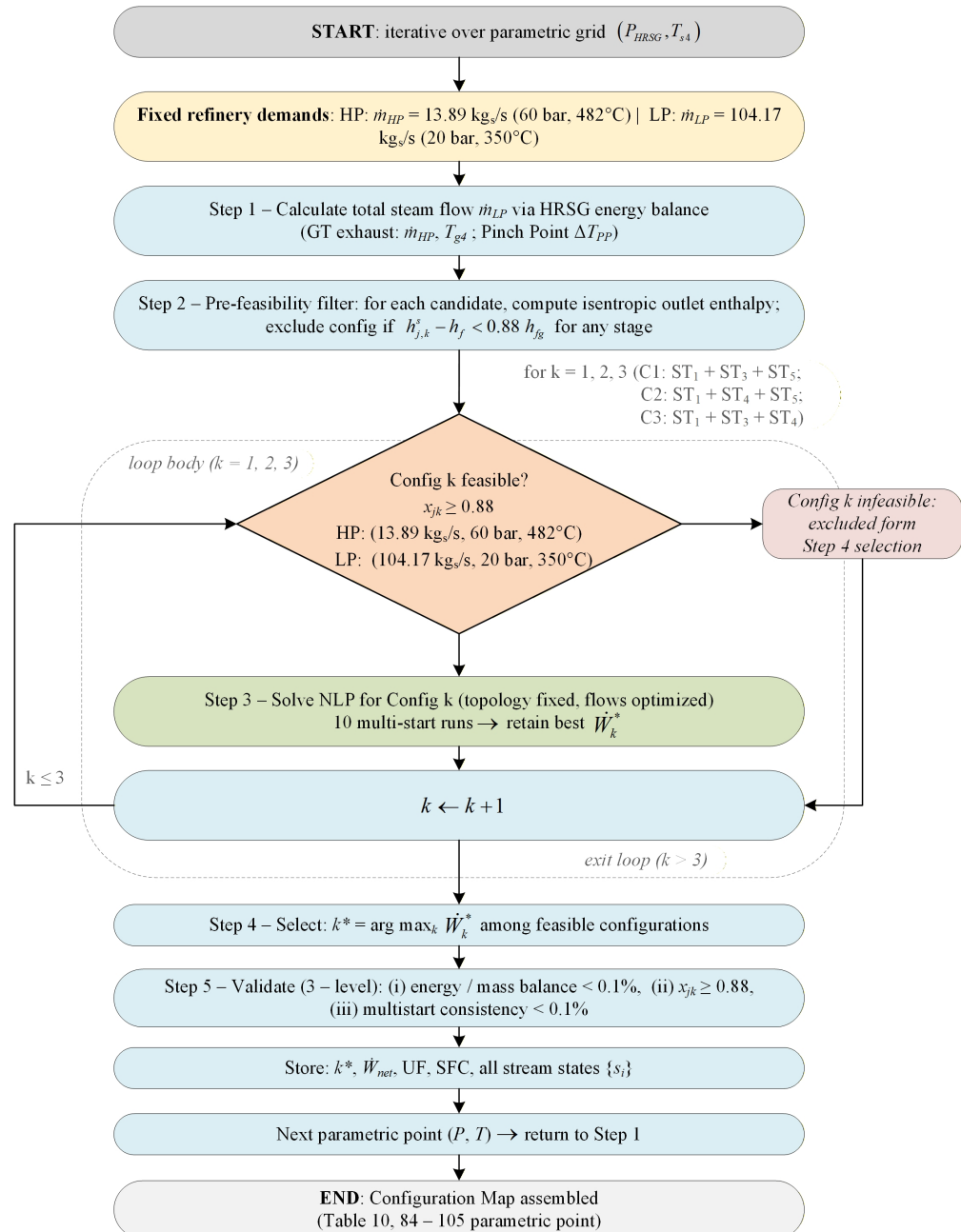


Figure 6. Flowchart of the proposed methodology for the optimization of the superstructure.

5. Results and Discussion

This section presents the optimal configurations identified through the optimization procedure described in Section 4. Analysis is organized into five subsections that progressively characterize the system: first the baseline reference without cogeneration is established, subsequently the three optimal configurations emerging from parametric analysis are identified, their individual thermodynamic behaviors are characterized, physical

mechanisms causing discrete transitions between configurations are explained, and finally multiple criteria are evaluated to recommend practical implementation.

5.1. Reference System and Identified Optimal Configurations

All results in this section represent locally optimal solutions within the enumerated configuration set; global optimality across all 2^{24} binary combinations is not guaranteed (Section 4.3).

5.1.1. Base Configuration Without Power Generation

The base system, described in Section 2.5 and shown in Figure 2, operates exclusively through isenthalpic expansion valves to satisfy refinery steam demands. This configuration represents the lower performance bound of the integrated turbine-process system. Valves EV_1 to EV_4 reduce steam pressure from HRSG level to HP and LP levels through irreversible processes. Tempering mixtures in headers Head HP and Head LP combine superheated and saturated steam streams to reach specified temperatures of $T_{HP} = 482\text{ }^{\circ}\text{C}$ and $T_{LP} = 350\text{ }^{\circ}\text{C}$, respectively.

Thermodynamic analysis of the base system reveals that throttling processes generate significant exergy destruction. For expansion valves, entropy generation is

$$\dot{S}_{\text{gen,EV}} = \dot{m}(s_{\text{out}} - s_{\text{in}}) > 0 \quad (33)$$

where outlet specific entropy $s_{\text{out}} > s_{\text{in}}$ due to isenthalpic process irreversibility. This entropy generation represents opportunity for power generation through turbine installation that utilizes available pressure differentials.

5.1.2. Quantitative Configuration Comparison

Systematic exploration of parametric space (P_{HRSG}, T_{s_4}) through the MINLP model formulated in Section 4.3 identifies three topologically distinct configurations that emerge as optimal under different HRSG operating conditions. Table 9 presents comprehensive quantitative comparison between the base system and the three cogeneration configurations.

The maximum power within Configuration 1's valid region is 78.96 MW at $P_{\text{HRSG}} = 140\text{ bar}$, $T_{s_4} = 500\text{ }^{\circ}\text{C}$ (Table 4), not at nominal conditions ($88.26\text{ bar}/510\text{ }^{\circ}\text{C} \rightarrow 72.32\text{ MW}$, 91.6 % of the maximum). For Configuration 2, the maximum is 73.22 MW at $75\text{ bar}/510\text{ }^{\circ}\text{C}$.

The base system operates with utilization factor $UF = 0.640$ and specific fuel consumption $SFC = 0.259\text{ kg/kWh}$, characteristic values of systems without steam cycle power generation potential utilization. The three cogeneration configurations increase utilization factor between 11.09% and 13.90%, simultaneously reducing specific fuel consumption between 20.01% and 22.39% compared to base system without cogeneration. These results quantify thermodynamic benefits of turbine-process integration and demonstrate that cogeneration represents an effective strategy for improving overall refinery energy system efficiency.

Differences among the three configurations are notable. Configuration 1 presents the widest operating range, maintaining feasibility for pressures between 75 and 140 bar and temperatures between 500 and 520 $^{\circ}\text{C}$. Configuration 2 exhibits a restricted range, limited to pressures between 75 and 110 bar for the same temperature interval. Configuration 3 operates exclusively in a high-temperature regime (550–560 $^{\circ}\text{C}$) but covers the entire evaluated pressure range. Generated power varies between 71.72 MW (Configuration 2, nominal conditions) and 80.82 MW (Configuration 3, optimal conditions), representing 12.7% difference, justifying a detailed analysis of each topology. The thermodynamic state properties for the three optimal configurations are shown in Appendix A, Tables A1–A4.

Table 9. Comparison between base system and cogeneration configurations at nominal conditions.

Parameter	Unit	Base System	Optimal Configuration		
			1	2	3
HRSG operating conditions					
P_{HRSG}	bar	88.26	88.26	88.26	140.0
T_{s_4}	°C	510	510	510	550
Validity region (pressure)	bar		75–140	75–110	70–140
Validity region (temperature)	°C		500–520	500–520	550–560
Active superstructure components					
Active headers		I, II	I, II	I	I, II
Active turbines			ST ₁ , ST ₃ , ST ₅	ST ₁ , ST ₄ , ST ₅	ST ₁ , ST ₃ , ST ₄
Number of expansion stages		0	3	3	4
System mass flows					
$\dot{m}_T$	kg/s	163.74	163.74	163.74	163.74
$\dot{m}_{\text{HP}}$	kg/s	13.89	13.89	13.89	13.89
$\dot{m}_{\text{LP}}$	kg/s	104.17	104.17	104.17	104.17
$\dot{m}_{\text{EX}}$	kg/s	45.68	45.68	45.68	45.68
Energy performance at nominal conditions					
$\dot{W}_{\text{ST}}$	MW	0	72.32	71.72	78.96
$\dot{W}_{\text{CC}}$	MW	288.0	360.32	359.72	366.96
UF		0.640	0.710	0.709	0.729
SFC	kg/kWh	0.259	0.207	0.208	0.201
Optimal performance within validity region					
$\dot{W}_{\text{ST,max}}$	MW	0	78.96	73.22	80.82
Conditions for maximum power			140/500	75/510	140/550
x_{min} in valid region			0.910	0.925	0.880
Improvement over base system					
$\Delta \dot{W}_{\text{ST}}$	MW		+72.32	+71.72	+78.96
ΔUF	%		+11.09	+10.93	+13.90
SFC reduction	%		−20.01	−19.69	−22.39

The utilization factor and specific fuel consumption are defined as

$$UF = \frac{\dot{W}_{\text{CC}} + \dot{Q}_{\text{proc}}}{\dot{m}_f \cdot LHV}, \quad \dot{Q}_{\text{proc}} = \sum_j \dot{m}_j (h_j - h_0), \quad h_0 = 125.74 \text{ kJ/kg}, \quad SFC = \frac{\dot{m}_f}{\dot{W}_{\text{CC}}}. \quad (34)$$

5.1.3. Configuration Performance Map in Parametric Space

Table 10 presents the complete map of optimal configurations identified for each evaluated combination of pressure P_{HRSG} and temperature T_{s_4} . This map constitutes one of the work's central results, revealing that the configuration generating maximum power is not unique but varies discretely according to HRSG operating conditions.

The map reveals three important structural characteristics. First, Configuration 1 dominates parametric space, occupying the most extensive region spanning pressures from 70 to 140 bar for temperatures between 500 and 520 °C, plus high-pressure zones (greater than 110 bar) for temperatures of 530 and 540 °C. Second, Configuration 2 emerges only in a narrow low-pressure zone (75–110 bar) for moderate temperatures (500–520 °C), coexisting with Configuration 1 in some parametric combinations. Third, Configuration 3 activates exclusively for high-temperature regime ($T_{s_4} \geq 550$ °C), occupying entire pressure range for $T_{s_4} = 550$ and 560 °C, plus penetrating toward lower temperatures (530 and 540 °C) in low-pressure region.

Table 10. Configuration performance map showing which of three candidate topologies generates maximum power at each HRSG operating point (locally optimal solutions identified through configuration enumeration).

T_{s4} (°C)	P_{HRSG} (Bar)								
	70	75	88.26	90	100	110	120	130	140
560	71.97	72.35	73.22	74.14	75.34	76.33	77.32	78.34	79.45
550	73.21	73.49	74.47	75.40	76.61	77.62	78.63	79.69	80.82
540	74.44	74.85	75.70	76.63	77.87	78.89	73.51	74.46	75.46
530	75.65	75.89	76.91	77.85	72.59	73.54	74.48	75.44	76.45
520	70.17	70.82	71.42	72.33	73.51	74.46	75.40	76.37	77.39
					71.22	70.46			
510	71.09	71.72	72.32	73.22	74.39	75.33	76.27	77.22	78.23
		73.83	71.72	70.76					
500	71.97	72.59	73.18	74.06	75.21	76.13	77.05	77.98	78.96
		72.21	70.12	69.16					

Note: Green cells (Config 2) in lower rows show Config 2 power at points where Config 1 is optimal (upper red cell), illustrating performance difference between configurations at same operating point. Colors indicate which configuration maximizes power at each point: Config 1 (red), Config 2 (green), Config 3 (blue). Values in MW.

Transitions between configurations occur at specific thresholds not evident through conventional thermodynamic analysis. For example, for fixed temperature $T_{s4} = 530$ °C, the system operates with Configuration 3 for pressures below 100 bar but abruptly transitions to Configuration 1 when pressure exceeds this threshold. Similarly, for fixed pressure $P_{HRSG} = 110$ bar, the Configuration 1 to Configuration 3 transition occurs between $T_{s4} = 520$ and 530 °C. Physical mechanisms causing these discrete transitions are analyzed in detail in Section 5.3.

5.2. Topological and Thermodynamic Analysis of Configurations

This subsection characterizes the three optimal configurations identified, describing their topology, analyzing their thermodynamic behavior through temperature–entropy diagrams, and quantifying their sensitivity to variations in HRSG operating parameters.

5.2.1. Configuration 1: System with Tempering via Valves

Figure 7 shows the topology of Configuration 1. The system activates headers Head I and Head II, allowing distribution of both superheated steam and saturated steam from the HRSG drum. Expansion valves EV_1 , EV_2 , and EV_3 remain operational, providing alternative routes for generating tempering streams. In terms of steam turbines, ST_1 , ST_3 , and ST_5 are activated, corresponding to three expansion stages that exploit the pressure differentials available between HRSG, HP, LP, and COND levels.

High-pressure steam flow is generated through mixing of three streams in the Head HP header. The first stream comes from expansion in the first stage of ST_1 , which reduces pressure from P_{HRSG} to $P_{HP} = 60$ bar. The second stream results from throttling in valve EV_1 , which brings superheated steam from Head I to the HP pressure level. The third stream, generated through throttling in EV_3 , transports saturated steam from Head II to the HP header. This last valve provides critical flexibility for tempering: when the outlet temperature of ST_1 exceeds the required temperature in Head HP ($T_{HP} = 482$ °C), the flow through EV_3 increases to reduce the mixture temperature through injection of relatively cold saturated steam.

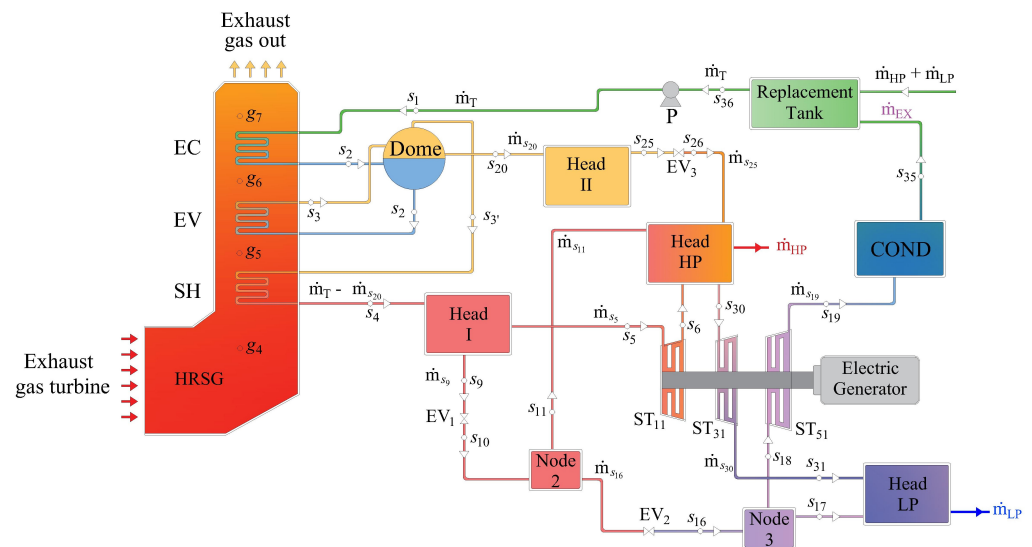


Figure 7. Topology of Configuration 1 showing active components: headers Head I and Head II, valves EV_1 – EV_3 , and turbines ST_1 , ST_3 , ST_5 with three total expansion stages.

Low-pressure steam flow is generated analogously. Excess steam from the Head HP header expands in the first stage of ST_3 until reaching pressure $P_{LP} = 20$ bar, feeding the Head LP header. This stream mixes with throttled steam in valve EV_2 , coming from node 3, adjusting the mixture temperature to meet the specification $T_{LP} = 350$ °C. Finally, excess steam from node 3 expands in turbine ST_5 to condensing pressure P_{COND} , generating additional power and closing the thermodynamic cycle.

Figure 8 presents the complete thermodynamic analysis of Configuration 1. The temperature–entropy diagram (a) under nominal conditions ($P_{HRSG} = 88.26$ bar, $T_{s_4} = 510$ °C) illustrates the multiple thermodynamic routes available in the superstructure. Expansion in ST_1 from state s_5 (superheated steam at 88.26 bar, 510 °C) to state s_6 (60 bar) generates the first power contribution. Isenthalpic processes in EV_1 and EV_3 are represented by vertical lines connecting the HRSG and HP pressure levels, illustrating the characteristic irreversibility of these valves. Mixing of the three streams in Head HP produces the HP steam flow state, identified by the red point at 60 bar and 482 °C.

Similarly, expansion in ST_3 from Head HP to the LP level, followed by mixing with steam from EV_2 , generates the LP steam flow identified by the blue point at 20 bar and 350 °C. Final expansion in ST_5 brings excess steam to the condenser, reaching quality $x_{s_8} = 0.935$ at state s_8 . This value is comfortably above the safety limit $x = 0.88$, indicated by the dashed line in the diagram, guaranteeing operation without risk of blade erosion.

Parametric sensitivity analysis for Configuration 1 is presented in Figure 8b. The generated power surface $\dot{W}_{ST}$ shows increasing trend with increments in HRSG pressure for fixed temperature. This behavior is explained by two competing effects. On one hand, higher pressure increases the pressure drop available for expansion in turbines, increasing specific work per unit mass of steam. On the other hand, higher pressure slightly reduces the generated steam flow $\dot{m}_T$ due to pinch point restrictions in the evaporator. The first effect dominates, resulting in net power increase.

For fixed pressure, temperature increments T_{s_4} produce the opposite effect: generated power decreases. This apparently counterintuitive behavior is due to higher superheat temperature requiring greater heat transfer in the superheater, reducing the energy available for evaporation and consequently decreasing total steam flow $\dot{m}_T$. The reduction in mass flow exceeds the increase in specific work from higher inlet enthalpy, resulting in lower net power.

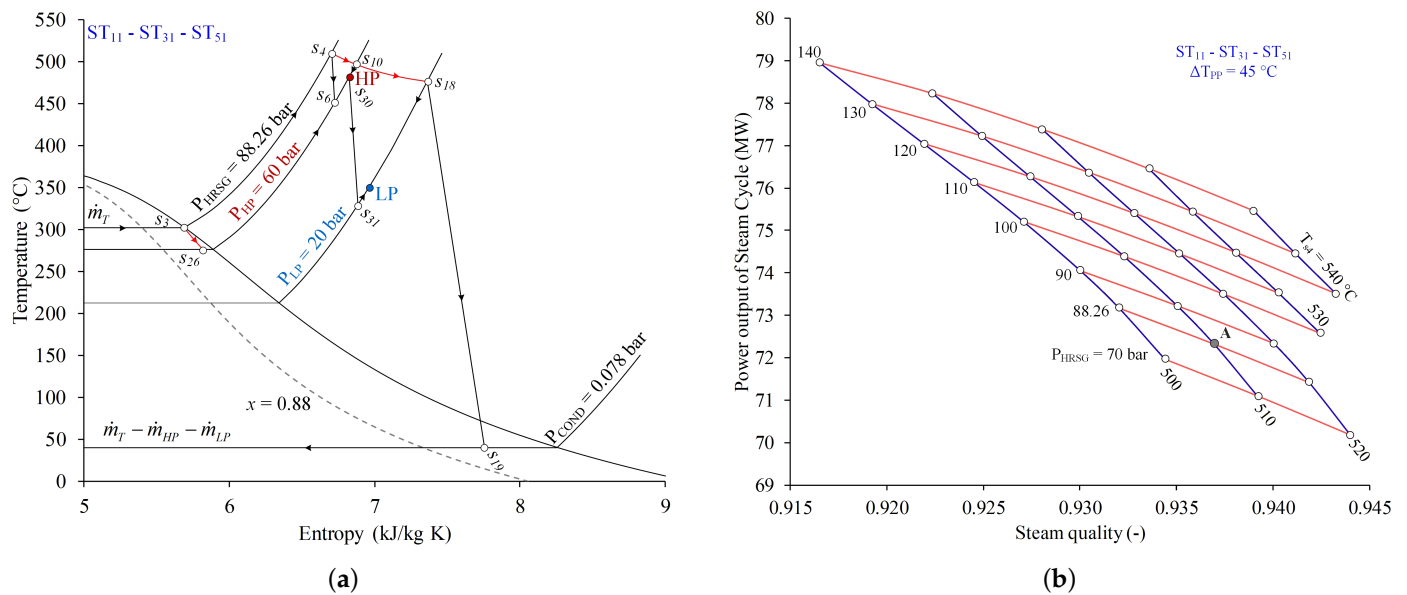


Figure 8. Configuration 1: (a) Temperature–entropy diagram showing expansion routes and mixing in HP and LP headers under nominal conditions ($P_{HRSG} = 88.26$ bar, $T_{s4} = 510$ °C); (b) Generated power surface and steam quality as function of HRSG parameters.

The optimal combination within Configuration 1's validity region is $P_{HRSG} = 140$ bar and $T_{s4} = 500$ °C, generating maximum power of 78.96 MW with steam quality $x_{min} = 0.910$ in the condenser. Under nominal operating conditions ($P_{HRSG} = 88.26$ bar, $T_{s4} = 510$ °C), the system generates 72.32 MW, representing 92.3% of maximum potential. This proximity indicates that nominal conditions are close to the thermodynamic optimum within the safe operating range.

5.2.2. Configuration 2: Simplified System Without Drum Steam

Configuration 2, shown in Figure 9, presents simplified topology compared to Configuration 1. Header Head II is deactivated, eliminating the distribution route for saturated steam from the HRSG drum. Consequently, valve EV_3 is also deactivated, since its specific function was to transport saturated steam for tempering. The system operates only with header Head I and valves EV_1 and EV_2 , distributing exclusively superheated steam from the superheater.

In terms of steam turbines, the configuration activates ST_1 , ST_4 , and ST_5 . The key difference from Configuration 1 lies in the substitution of ST_3 by ST_4 . While ST_3 initiates its expansion from the Head HP header, turbine ST_4 initiates from node 2, expanding steam directly from the HP level to LP without intermediate extraction of the stream feeding Head HP.

High-pressure steam flow is obtained through mixing of only two streams in Head HP. The first is superheated steam from node 2 after partial throttling, which acts as the hot stream. The second is steam expanded in the first stage of ST_1 from P_{HRSG} to P_{HP} , which typically is at a temperature lower than $T_{HP} = 482$ °C and acts as the cold stream. The absence of valve EV_3 eliminates the possibility of tempering through saturated steam, significantly limiting system flexibility.

Similarly, low-pressure steam flow is generated through the mixing of two streams. The first comes from throttling in EV_2 , transporting superheated steam from node 3 as the hot stream. The second results from expansion in the first stage of ST_4 , which reduces pressure from P_{HP} to P_{LP} . The outlet temperature of this expansion, denoted as T_{s13} , determines the feasibility of the complete configuration.

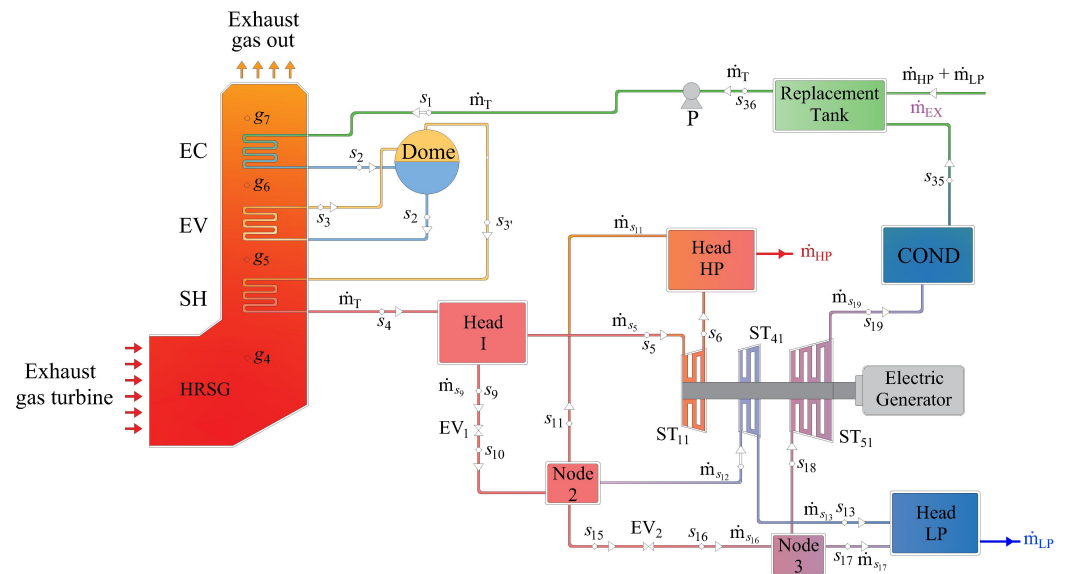


Figure 9. Topology of Configuration 2 showing simplification with respect to Config. 1: only header Head I active, valves EV₁ and EV₂, turbines ST₁, ST₄, ST₅.

The temperature–entropy diagram of Configuration 2 (Figure 10a) reveals the critical restriction that limits its operating range. The outlet temperature of ST₄ at state s_{13} must obligatorily satisfy $T_{s13} < T_{LP} = 350$ °C so that mixing with steam from EV₂ can reach the specified temperature of the LP header. For nominal conditions, $T_{s13} = 332$ °C, providing margin of only 18 °C with respect to the limit. This narrow margin makes the configuration sensitive to variations in HRSG operating parameters.

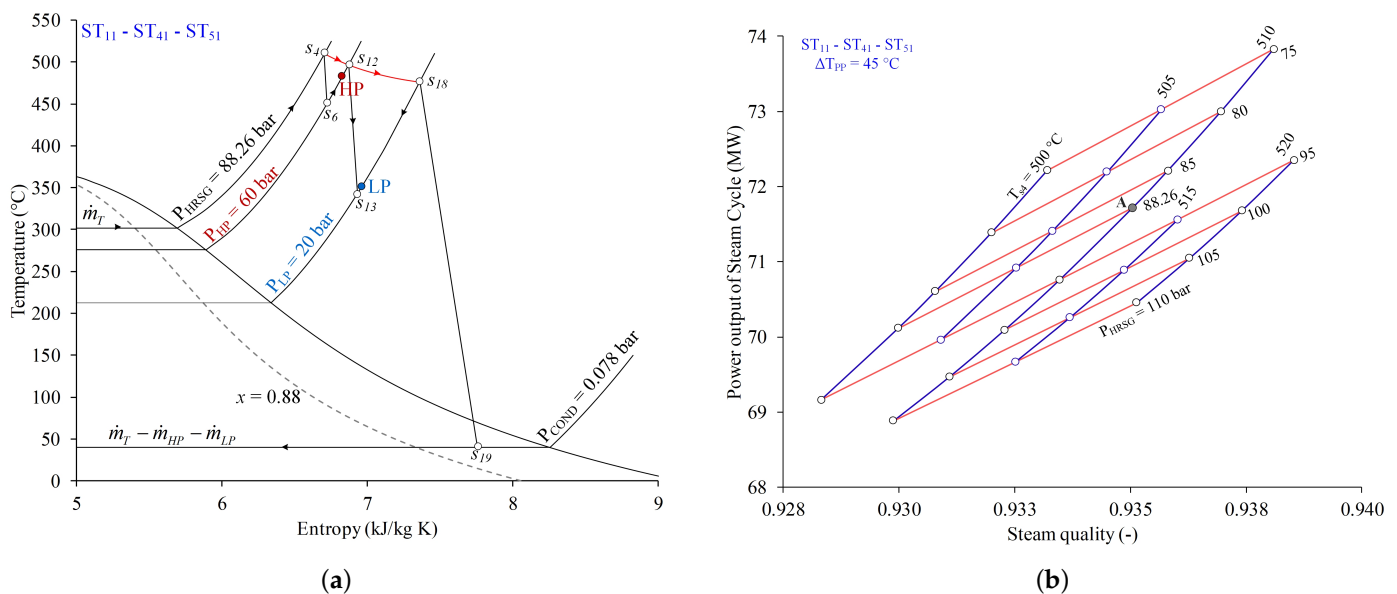


Figure 10. Configuration 2: (a) T-s diagram showing critical restriction $T_{s13} < T_{LP}$ that limits operating range; (b) Power surface exhibiting inverse trend to Config. 1 (power decreases with pressure).

Parametric sensitivity of Configuration 2, presented in Figure 10b, exhibits opposite behavior to Configuration 1. For fixed temperature, increments in pressure P_{HRSG} reduce generated power. This counterintuitive behavior is explained through analysis of the restriction $T_{s13} < T_{LP}$. The outlet temperature of expansion in ST₄ increases when inlet pressure P_{HP} increases, because the specific entropy of steam in Head HP decreases with higher pressure at fixed temperature. By increasing P_{HRSG} , this effect propagates toward

Head HP, increasing T_{s13} and approaching it dangerously to the 350 °C limit. To maintain feasibility, the optimizer reduces flows through ST_4 , decreasing power generation.

The validity region of Configuration 2 is limited to pressures between 75 and 110 bar and temperatures between 500 and 520 °C. Maximum power of 73.22 MW is reached at the lower pressure limit ($P_{HRSG} = 75$ bar, $T_{s4} = 510$ °C), where the restriction $T_{s13} < T_{LP}$ is most relaxed. Under nominal conditions, the configuration generates 71.72 MW, representing 1.18 MW less than Configuration 1 for the same HRSG operating conditions. The bounded feasibility region reflects a thermodynamic boundary, not a numerical artifact: the equality constraint $T_{LP} = 350$ °C cannot be met when $h_{s13} \geq 3137.64$ kJ/kg, creating a sharp—not gradual—transition at the feasibility boundary (Section 5.3.1).

5.2.3. Configuration 3: High-Power System with Multi-Stage Expansion

Configuration 3, presented in Figure 11, represents the most complex topology of the three identified. Similar to Configuration 1, it activates both headers Head I and Head II, in addition to valves EV_1 , EV_2 , and EV_3 . The distinctive difference lies in activation of both expansion stages of turbine ST_4 , allowing complete expansion route $HP \rightarrow LP \rightarrow COND$. This feature enables operation at elevated temperatures while maintaining acceptable steam quality in the condenser.

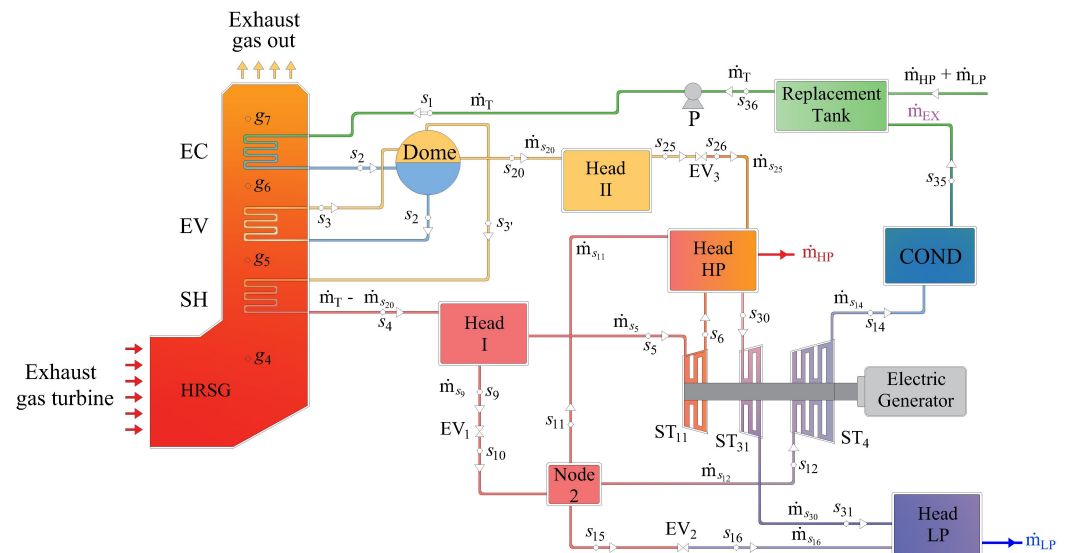


Figure 11. Topology of Configuration 3 showing maximum complexity: both headers active, all valves, and four total expansion stages including both stages of ST_4 .

The set of active turbines includes ST_1 , ST_3 , and ST_4 , totaling four expansion stages: the first stage of ST_1 ($HRSG \rightarrow HP$), the first stage of ST_3 ($HP \rightarrow LP$), and both stages of ST_4 ($HP \rightarrow LP$ followed by $LP \rightarrow COND$). This multiplicity of routes provides superior flexibility for distribution of mass flows between the different pressure levels, maximizing power generation subject to demand and steam quality restrictions.

High-pressure steam flow is generated through the same three-stream scheme as Configuration 1: steam expanded in ST_1 , throttled steam in EV_1 , and saturated steam throttled in EV_3 . However, the relative proportions of these streams differ significantly due to high-temperature conditions. Figure 12 illustrates two distinct operating regimes within Configuration 3's validity region.

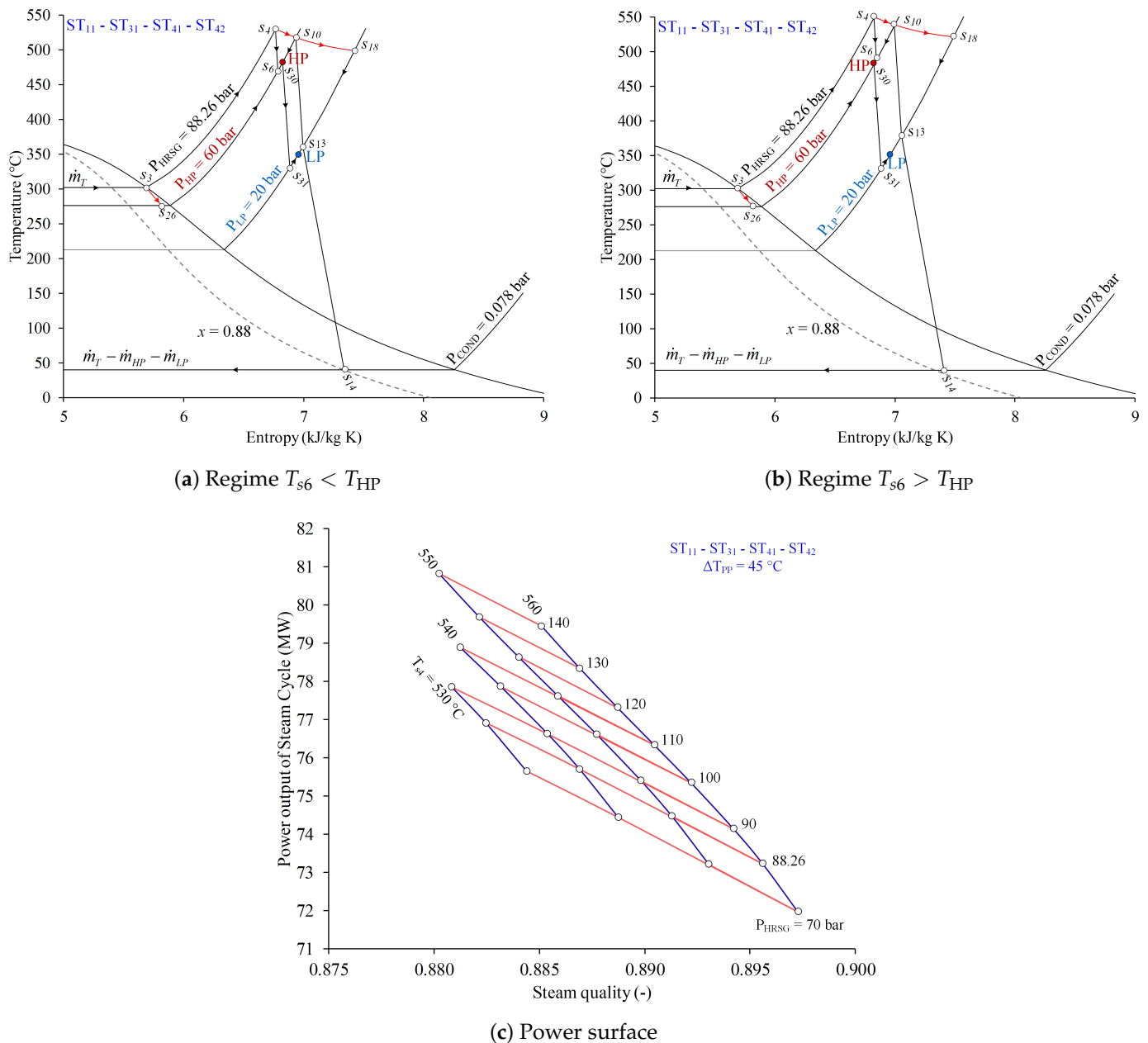


Figure 12. Configuration 3: (a,b) T-s diagrams showing two operating regimes according to outlet temperature of ST_1 relative to T_{HP} , demonstrating flexibility of tempering system; (c) Power generation for high-temperature range (550–560 °C) showing maxima of 80.82 MW but critical quality $x \approx 0.88$.

In regime (a), when the outlet temperature of ST_1 is lower than the HP header temperature ($T_{s6} < T_{HP} = 482$ °C), the system requires greater flow of the hot stream from EV_1 to elevate the mixture temperature. This regime typically occurs at the lower temperature limit of the validity region. In regime (b), when $T_{s6} > T_{HP}$ due to high superheat temperature, the system increases the flow of saturated steam from EV_3 to temper the mixture, reducing temperature to the specified value of 482 °C. This regime is characteristic of the upper temperature limit.

For low-pressure steam flow, the temperature of the cold stream from the first stage of ST_3 remains essentially constant since inlet conditions in Head HP are fixed by the demand specification. The flow of throttled steam in EV_2 adjusts the mixture temperature to satisfy $T_{LP} = 350$ °C. Excess steam expands in both stages of ST_4 , from the HP level to the condenser, generating significant contribution to total cycle power.

Power generation analysis for Configuration 3, presented in Figure 12c, reveals that this configuration reaches the highest power levels among the three evaluated. The power surface covers the temperature range 550–560 °C for all pressures, in addition to penetrating toward lower temperatures (530–540 °C) in the low-pressure region. Maximum power of 80.82 MW is obtained at conditions $P_{\text{HRSG}} = 140$ bar and $T_{s_4} = 550$ °C, representing 11.0% increase with respect to the nominal value of Configuration 1.

However, Configuration 3 operates with steam quality close to the critical limit. For maximum power conditions, quality at state s_{14} (outlet of the second stage of ST₄) reaches $x_{s_{14}} = 0.881$, barely 0.001 above the safety limit $x = 0.88$. The entire valid operating range maintains qualities between 0.880 and 0.900, significantly lower than the 0.910–0.935 margin of Configuration 1. This proximity to the limit demands rigorous operational monitoring and precise control systems to guarantee that transient variations in operating conditions do not lead to quality restriction violation.

5.3. Thermodynamic Mechanisms of Transitions Between Configurations

Two thermodynamic criteria govern the configuration map: (i) $h_{s_{13}} \geq 3137.64$ kJ/kg triggers Config. 2 → 1 (Section 5.3.1); (ii) $x_{s_{19}} > 0.940$ triggers Config. 1 → 3 (Section 5.3.2).

The configuration map presented in Table 10 reveals that transitions between high-performing identified configurations occur at specific thresholds of the parametric space (P_{HRSG}, T_{s_4}). These transitions are discrete: upon crossing a critical threshold, the system changes abruptly from one topological configuration to another without intermediate states. This phenomenon is not evident through conventional thermodynamic analysis and constitutes one of the central scientific contributions of the present work. This subsection develops causal analysis of transitions through rigorous characterization of active thermodynamic restrictions, demonstrating that thresholds correlate with systematic activation of thermodynamic constraints, which can be identified through evaluation of feasibility conditions.

5.3.1. Transition from Configuration 2 to Configuration 1

The first transition of interest occurs in the moderate temperature regime ($T_{s_4} = 500$ – 520 °C) when HRSG pressure exceeds values between 100 and 110 bar. As observed in Table 10, for fixed temperature $T_{s_4} = 520$ °C, the system operates with Configuration 2 for pressures between 75 and 100 bar, but transitions to Configuration 1 when pressure reaches 110 bar. This threshold varies slightly with temperature, but the causal mechanism remains invariant.

Analysis of Configuration 2 in Section 5.2.2 identified that the critical restriction is $T_{s_{13}} < T_{\text{LP}}$, where $T_{s_{13}}$ denotes the outlet temperature of the first stage of ST₄. This temperature is determined by pressure and enthalpy ($P_{\text{LP}}, h_{s_{13}}$) and through the expression for isentropic expansion with efficiency:

$$h_{s_{13}} = h_{s_{12}} - \eta_{\text{is}}(h_{s_{12}} - h_{s_{13s}}) \quad (35)$$

where $h_{s_{12}}$ is the inlet enthalpy to ST₄ (equal to the inlet enthalpy of EV₁, $h_{s_{12}} = h_{s_9}$), $\eta_{\text{is}} = 0.89$ is the isentropic efficiency of the turbine, and $h_{s_{13s}}$ is the enthalpy obtained through isentropic expansion from inlet conditions to outlet pressure $P_{\text{LP}} = 20$ bar.

The enthalpy $h_{s_{13s}}$ is calculated through the constant entropy condition:

$$s_{s_{13s}} = s_{12}, \quad P_{s_{13s}} = P_{\text{LP}} \quad (36)$$

where $s_{s_{13s}}$ is the specific entropy of steam coming from valve EV₁ and node 2. This entropy depends on conditions (P_{HRSG}, T_{s_4}). The mechanism causing the transition is explained through the effect of P_{HRSG} on the thermodynamic properties of steam in EV₁. When HRSG

pressure increases and T_{s4} is constant, the steam enthalpy (h_{s9} feeding EV_1) decreases. This implies that the enthalpy at the inlet of ST_4 is lower and temperature T_{s13} at the end of expansion moves below T_{LP} .

However, the dominant effect comes from the increase in superheat temperature T_{s4} . Although pressure P_{HRSG} remains fixed, higher temperature implies a greater increase in enthalpy h_{s4} , which consequently will result in higher temperature at the inlet and outlet of ST_4 .

The feasibility condition of Configuration 2 requires

$$T_{s13} < T_{LP} = 350\text{ }^{\circ}\text{C} \quad (37)$$

or equivalently, this implies that

$$h_{s13} < h_{LP} = 3137.64\text{ kJ/kg} \quad (38)$$

When P_{HRSG} exceeds the critical threshold, the system cannot operate with Configuration 2 because temperature T_{s13} would exceed $350\text{ }^{\circ}\text{C}$, making it impossible to generate LP steam flow through mixing. The optimizer detects this infeasibility and automatically changes to Configuration 1, which incorporates valve EV_3 for additional tempering through saturated steam injection. This valve relaxes the temperature restriction by providing an additional cold stream, enabling operation at higher pressures.

5.3.2. Transition from Configuration 1 to Configuration 3

The second transition of interest occurs in the elevated temperature regime ($T_{s4} \geq 530\text{ }^{\circ}\text{C}$) and varies its pressure threshold according to specific temperature. As observed in Table 10, for $T_{s4} = 530\text{ }^{\circ}\text{C}$, the transition occurs at $P_{HRSG} = 100\text{ bar}$: the system operates with Configuration 3 for pressures less than or equal to 90 bar, but changes to Configuration 1 for pressures from 100 bar onward. For $T_{s4} = 540\text{ }^{\circ}\text{C}$, the threshold increases to 120 bar. This behavior suggests that the causal mechanism involves interaction between both HRSG operating parameters.

Thermodynamic analysis reveals that the transition is related to the steam quality restriction in the final expansion to the condenser. For Configuration 1, excess steam coming from expansion valve EV_2 and from node 3, expands in turbine ST_5 from the LP level to condensing pressure. Quality in the condenser is determined by

$$x_{s19} = \frac{h_{s19} - h_f(P_{COND})}{h_{fg}(P_{COND})} \quad (39)$$

where h_{s19} is the specific enthalpy of steam at the outlet of ST_5 , $h_f(P_{COND})$ is the saturated liquid enthalpy, and $h_{fg}(P_{COND})$ is the heat of vaporization at condensing pressure.

When the superheat temperature T_{s4} increases for constant pressure P_{HRSG} , the inlet enthalpy to the steam system increases. Although total mass flow $\dot{m}_T$ decreases due to heat transfer restrictions in the HRSG, the specific enthalpy of steam in node 3 (inlet to ST_5) is the same, $h_{s4} = h_{s18}$. Then, this enthalpy increases due to a temperature increase in T_{s4} and propagates through the expansion, resulting in higher enthalpy h_{s8} in the condenser and consequently both higher steam quality x_{s19} and a decrease in power generation $\dot{W}_{ST}$.

In the opposite case, when pressure P_{HRSG} increases for constant superheat temperature T_{s4} , the inlet enthalpy to the steam system decreases. This causes an increase in steam generation in the HRSG, resulting in an increase in power generation $\dot{W}_{ST}$, and a decrease in steam quality x_{s19} .

The lowest quality $x_{s19} = 0.916$ in Configuration 1 is shown for operation at the highest pressure $P_{HRSG} = 140\text{ bar}$ and the lowest superheat temperature $T_{s4} = 500\text{ }^{\circ}\text{C}$. However,

this minimum quality, obtained from the set of possibilities (P_{HRSG}, T_{s4}) , is far from the allowed limit $x = 0.88$.

For elevated temperatures ($T_{s4} \geq 530$ °C) and pressures ($P_{HRSG} \geq 100$ bar), quality x_{s19} in Configuration 1 increases drastically $x_{s19} > 0.940$. This quality increase causes a decrease in power generation $\dot{W}_{ST}$ and, at the same time, an increase in heat rejection in the condenser $\dot{Q}_{COND}$.

Configuration 3 in addition to generating higher power than Configuration 1, solves the steam quality problem through division of the HP $\rightarrow$ COND expansion into two stages within ST₄. Steam expanding in the second stage of ST₄ to condensing pressure presents a quality x_{s14} that approaches dangerously close to the safety limit $x = 0.88$. This approach results when the temperature at the end of the first expansion T_{s13} is extremely close to temperature T_{LP} . This condition occurs under the condition of the highest pressure P_{HRSG} within the temperature range of superheat $T_{s4} = 530$ and 550 °C.

Although formally the configuration remains feasible while $x_{s14} > 0.88$, the reduced safety margin makes this configuration operationally risky. Transient variations in operating conditions could lead to momentary violation of the limit, causing risk of blade erosion.

The decision mechanism between Configuration 1 and Configuration 3 represents a trade-off between operational simplicity and power maximization. Configuration 1 uses three total expansion stages, while Configuration 3 requires four stages. This additional complexity is only justified when the steam quality restriction becomes sufficiently active. The transition threshold occurs when the benefit of higher power generation (due to higher steam flow available at high temperatures) compensates for the cost of increased operational complexity.

Quantitative prediction of the transition threshold is more complex than in the case of the Config. 2 $\rightarrow$ Config. 1 transition since it involves optimization of the balance between multiple objectives. However, qualitative analysis provides a clear criterion: the transition occurs when steam quality in Configuration 1 is greater than $x_{s19} > 0.940$ and with it a decrease in power generation. Power generation in Configuration 3 exceeds that of Configuration 1 by a significant margin (typically greater than 4 MW) with a steam quality margin of ($x_{s14} = 0.88 - 0.90$).

Validation is obtained through analysis of specific cases. For $P_{HRSG} = 100$ bar and $T_{s4} = 530$ °C, Configuration 1 generates 72.59 MW with $x_{s19} = 0.9424$, while Configuration 3 generates 77.85 MW with $x_{s14} = 0.8809$. The difference of 5.26 MW (7.24%) justifies the optimizer's preference for Configuration 3 despite having a decrease in safety margin in steam quality.

5.3.3. Implications for Design and Operation

The identified thermodynamic mechanisms have three important practical implications for design and implementation of cogeneration systems in refineries.

First, system optimization must be performed considering the complete parametric space (P_{HRSG}, T_{s4}) rather than a single nominal point. The existence of discrete transitions implies that the local optimum at a specific point may be significantly inferior to the global optimum achievable in another region of the parametric space with different topological configuration. Design must specify not only the nominal configuration but also valid operating ranges and alternative configurations available for different operating conditions.

Second, operational flexibility of the system is maximized by installing all superstructure components rather than only those corresponding to the nominally optimal configuration. This additional investment allows the system to adapt its active topology according to variable demand conditions and equipment availability, maintaining high efficiency in multiple operating scenarios. The decision between flexible design and specific

design should be evaluated through technical-economic analysis that quantifies the value of flexibility versus the incremental investment required.

Third, transition thresholds between configurations can be explained through systematic thermodynamic analysis of active restrictions. This mechanistic understanding allows anticipating changes in optimal configuration during the design phase, avoiding operational surprises and informing specification of control and monitoring systems. The characterization procedure developed in this subsection is generalizable to other cogeneration systems through application of the same conceptual framework: identify critical restrictions, analyze their variation with design parameters, and determine violation conditions.

5.3.4. Multi-Criteria Evaluation for Design Selection

Selection of the most appropriate configuration for implementation requires multi-criteria analysis that considers not only generated power but also operational flexibility, reliability, and system complexity. A weighted evaluation methodology is developed based on five quantitative criteria.

Table 11 defines the five evaluation criteria with their operational definitions and assigned weights. Weights were assigned using the Analytic Hierarchy Process (AHP, Saaty 1980) reflecting CFE-PEMEX industrial priorities: maximum power generation (0.25), operational flexibility (0.20), safety margin (0.20), maintenance complexity (0.15), and robustness (0.20). The sensitivity analysis (Table 13) confirms Configuration 1 is optimal in three of four scenarios under $\pm 50\%$ weight variation.

Table 11. Multi-criteria evaluation criteria with assigned weights.

Criterion	Weight	Operational Definition
C1: Maximum power	0.25	Maximum net power in validity region: $\dot{W}_{\text{net,max}}$ [MW]. Maximizes economic return.
C2: Operating range	0.20	Area of parametric region: $A = \Delta P_{\text{HRSG}} \times \Delta T_{s_4}$ [bar·°C]. Larger area indicates greater operational flexibility.
C3: Safety margin	0.20	Distance to critical limit: $\Delta x = x_{\text{min}} - 0.88$. Greater margin protects against blade erosion.
C4: Simplicity index	0.15	Inverse of expansion stages: $IS = 1/N_{\text{stages}}$. Higher index reduces maintenance costs.
C5: Robustness index	0.20	Inverse of standard deviation: $IR = 1/\sigma(\dot{W}_{\text{ST}})$ [MW ⁻¹]. Higher index improves operational thermodynamic consistency.

Note: All criteria are defined so that higher value indicates better performance. The validity region is the set of points (P_{HRSG}, T_4) where the configuration maximizes power while meeting thermodynamic restrictions.

The validity regions of configurations are determined through exhaustive parametric analysis. For each combination of HRSG conditions (P_{HRSG}, T_4) within the range of interest (70–140 bar, 500–560 °C), the topological optimization problem is solved to identify which configuration maximizes net power while meeting all thermodynamic restrictions. From this analysis naturally emerges the partition of the parametric space: each point belongs to the validity region of the configuration that is superior there. For example, Configuration 1 presents a validity region in the range 70–140 bar and 500–530 °C, which means that at any point within those ranges, Configuration 1 generates higher power than the alternatives while meeting restrictions.

All criteria are consistently defined so that a higher value indicates better performance. For criteria C1–C3, this is direct (higher power, larger range, and greater margin are preferable), while for C4 and C5 inverse indices are used: a higher simplicity index corresponds

to fewer stages (simpler), and a higher robustness index corresponds to lower standard deviation (more robust).

Normalization of each criterion is performed through

$$v_{i,k} = \frac{\text{value}_{i,k}}{\max_j(\text{value}_{j,k})} \quad (40)$$

where i identifies the configuration being evaluated ($i = 1, 2, 3$ for Config 1, Config 2, Config 3), k identifies the criterion being normalized ($k = 1, 2, 3, 4, 5$ for C1 to C5), and $\max_j(\text{value}_{j,k})$ represents the maximum value of criterion k among all configurations, where j traverses the three configurations ($j = 1, 2, 3$). For example, to normalize criterion C2 (operating range) of Config 1, we calculate $v_{1,2} = \text{value}_{1,2} / \max(\text{value}_{1,2}, \text{value}_{2,2}, \text{value}_{3,2})$, i.e., divide Config 1's range by the maximum range observed in the three configurations. This normalization produces values $v_{i,k} \in [0, 1]$ where $v_{i,k} = 1$ indicates that configuration i presents the best performance for the criterion k .

The total weighted score for each configuration is calculated through

$$S_i = \sum_{k=1}^5 w_k \cdot v_{i,k} \quad (41)$$

where w_k is the weight of criterion k (Table 11) and $\sum_{k=1}^5 w_k = 1$. The configuration with the highest score S_i is considered superior according to this multi-criteria analysis.

Table 12 presents the comparative evaluation of the three optimal configurations identified. The raw values of each criterion are determined through exhaustive analysis over the validity regions of each configuration.

Table 12. Multi-criteria evaluation of identified configurations.

Evaluation Criterion	Weight	Config. 1	Config. 2	Config. 3
C1: Maximum power Absolute value (MW)	0.25	78.97	73.23	80.82
Normalized evaluation		0.977	0.906	1.000
C2: Operating range Parametric area (bar·°C)	0.20	1365	462	1050
Normalized evaluation		1.000	0.338	0.769
C3: Safety margin $\Delta x = x_{\min} - 0.88$	0.20	0.030	0.045	0.001
Normalized evaluation		0.667	1.000	0.022
C4: Simplicity index $IS = 1/N_{\text{stages}}$	0.15	0.333	0.333	0.250
Normalized evaluation		1.000	1.000	0.750
C5: Robustness index $IR = 1/\sigma$ (MW ⁻¹)	0.20	0.455	0.714	0.444
Normalized evaluation		0.637	1.000	0.622
Weighted score	1.00	0.855	0.844	0.645
Recommendation		Base design	Limited	Future expansion

Note: Normalized evaluation on 0–1 scale, where 1 represents best performance. All criteria are defined so that higher value indicates better performance.

Configuration 3 reaches 80.82 MW, establishing the normalization reference. Configuration 1 achieves 97.7% of this maximum value (78.97 MW), while Configuration 2 reaches

90.6% (73.23 MW). The assigned weight of 0.25 reflects that, although important, power is not the only determining criterion.

Configuration 1 covers 1365 bar·°C, while Configuration 2 only spans 462 bar·°C. Configuration 3 occupies intermediate position with 1050 bar·°C. The area of each region is calculated by counting parametric points where the configuration is optimal, multiplied by mesh spacing ($\Delta P \times \Delta T$). The weight of 0.20 recognizes that operational flexibility is critical for system robustness against uncertainties.

Configuration 2 offers greater margin (0.045), followed by Configuration 1 (0.030), while Configuration 3 operates dangerously close to the limit (0.001). This criterion receives weight of 0.20 due to reliability and maintenance cost implications associated with operation near erosion limits.

Configurations 1 and 2 require three stages ($IS = 0.333$), while Configuration 3 requires four stages ($IS = 0.250$). The relatively lower weight (0.15) reflects that moderately greater complexity may be justified if other benefits are significant.

Configuration 2 presents greater robustness ($IR = 0.714 \text{ MW}^{-1}$, equivalent to $\sigma = 1.40 \text{ MW}$), followed by Configuration 1 ($IR = 0.455 \text{ MW}^{-1}$, $\sigma = 2.20 \text{ MW}$), while Configuration 3 exhibits lower robustness ($IR = 0.444 \text{ MW}^{-1}$, $\sigma = 2.25 \text{ MW}$). The standard deviation is calculated over the set of powers generated at all parametric points of the validity region. For example, Configuration 2 with $\sigma = 1.40 \text{ MW}$ experiences typical variation of $\pm 1.40 \text{ MW}$ when operating at different points in its validity region. The weight of 0.20 recognizes the importance of performance thermodynamic consistency for operational planning.

The total weighted score, calculated through Equation (41), positions Configuration 1 as superior with 0.82 points. This configuration offers optimal balance between power generation (97.7% of absolute maximum), extensive operating range (100% of maximum), adequate safety margin (67% of maximum), competitive simplicity (100%), and acceptable operational robustness (64% of best). Configuration 3 reaches 0.69 points, penalized mainly by critical safety margin (2% of best) and lower robustness (62%). Configuration 2 obtains 0.68 points, limited by reduced power (91%) and narrow operating range (34% of maximum).

5.3.5. Sensitivity Analysis of Multi-Criteria Evaluation

Robustness of the recommended selection is verified through sensitivity analysis that evaluates the effect of changes in weights assigned to each criterion. Table 13 presents total scores under three alternative weighting scenarios.

Table 13. Sensitivity analysis: total score under different weighting schemes.

Weighting Scenario	Weights [C1–C5]	Config. 1	Config. 2	Config. 3	Optimal
Base (Table 12)	[0.25, 0.20, 0.20, 0.15, 0.20]	0.82	0.68	0.69	1
Emphasis on maximum power	[0.40, 0.15, 0.15, 0.15, 0.15]	0.85	0.71	0.77	1
Emphasis on reliability	[0.15, 0.10, 0.30, 0.15, 0.30]	0.74	0.83	0.52	2
Emphasis on flexibility	[0.20, 0.35, 0.15, 0.10, 0.20]	0.87	0.62	0.73	1

The analysis reveals that Configuration 1 maintains its superior position in three of the four evaluated scenarios. In the base scenario, Configuration 1 obtains 0.82 points, clearly surpassing alternatives. When the weight of maximum power is increased to 0.40, Configuration 1 improves its score to 0.85, although Configuration 3 increases competitiveness (0.77 points) due to its higher absolute power. However, Configuration 1 maintains advantage due to its superior balance in other criteria.

In the scenario with extreme emphasis on reliability (weights of 0.30 for safety margin and robustness), Configuration 2 emerges as superior (0.83 points), surpassing Configura-

tion 1 (0.74 points). This occurs because Configuration 2 presents the best safety margin (0.045) and lowest variability ($\sigma = 1.40$ MW). Configuration 3 is severely penalized in this scenario (0.52 points) due to its critical margin of barely 0.001.

When flexibility is emphasized by increasing the weight of operating range to 0.35, Configuration 1 reaches its best relative performance (0.87 points), leveraging its wide validity region of 1365 bar·°C. Configuration 2 is particularly affected in this scenario (0.62 points) due to its restricted validity region of only 462 bar·°C.

The robustness of Configuration 1 as a superior option is confirmed by maintaining first place in three of four scenarios. Configuration 2 would only be justified in contexts where reliability (safety margin and operational robustness) is absolutely prioritized over flexibility and power. However, such an extreme scenario is unlikely in real industrial applications, where balance between multiple objectives is generally preferable.

5.3.6. Sensitivity of Steam Turbine Isentropic Efficiency

The isentropic efficiency of steam turbines is a determining parameter in the thermodynamic performance of the cycle, as it directly influences power generation and steam quality at the end of each expansion. Figure 13 presents a sensitivity analysis of Configuration 1, evaluating power generation and minimum steam quality as a function of P_{HRSG} and T_{s4} for two values of η_{IST} : the nominal (0.89) and a reduced one (0.85). The latter simulates operational wear conditions on the turbine blades.

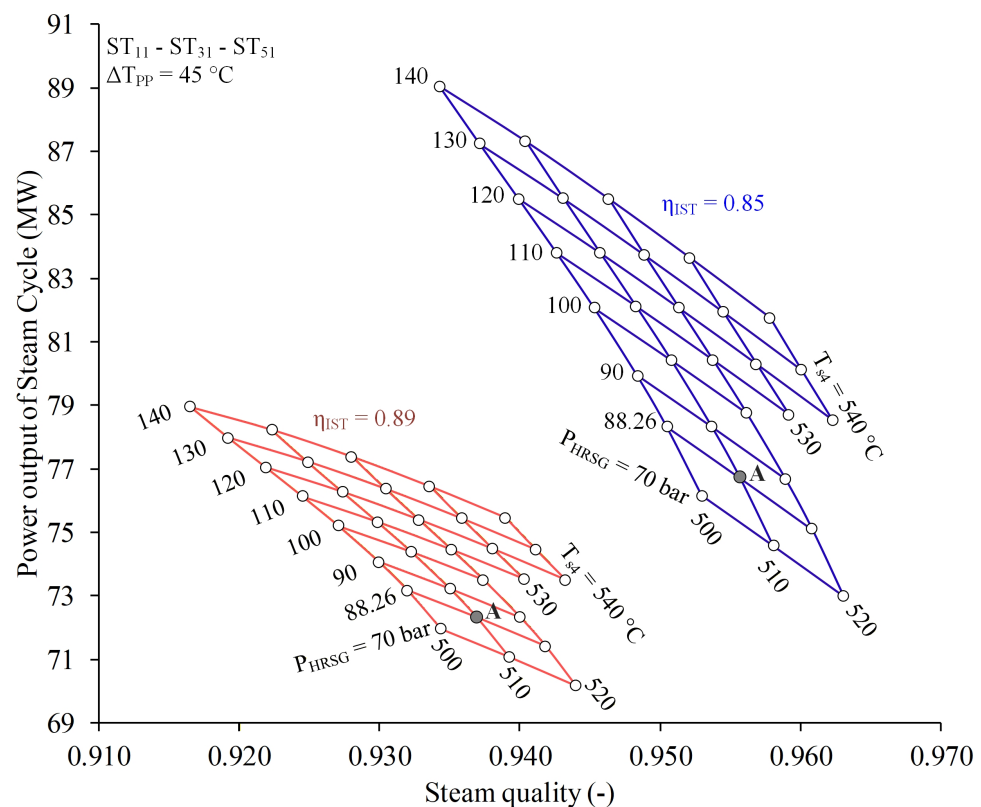


Figure 13. Configuration 1: Power generation and steam quality as function of P_{HRSG} , T_{s4} at $\eta_{IST} = 0.89$ and 0.85.

Formally, reducing η_{IST} affects steam quality through $h_{out} = h_{in} - \eta_{IST}(h_{in} - h_{out,s})$ (enthalpy increases) and $x_{out} = (h_{out} - h_f)/h_{fg}$ (quality increases), allowing the optimizer to route more flow to condenser expansion without violating $x \geq 0.88$.

The figure reveals a notable result: a lower isentropic efficiency ($\eta_{IST} = 0.85$) leads to higher power generation values across the entire parametric range compared to the

nominal condition. This seemingly counterintuitive behavior is explained by the interaction between expansion thermodynamics and the response of the MINLP optimizer. While a reduced η_{IST} decreases the specific work per stage, it also increases the enthalpy of the remaining steam, allowing the optimizer to reallocate mass flows toward the expansion routes that maximize net power within the superstructure, favoring a greater flow rate expanded to the condenser.

Despite this quantitative change in power, the optimal topology (Configuration 1) remains unaltered. The power surface for $\eta_{IST} = 0.85$ is approximately parallel to that for $\eta_{IST} = 0.89$ but shifted toward higher values. This confirms the robustness of Configuration 1 against degradation in turbine efficiency, a relevant factor for long-term operation.

Additionally, it is observed that the lower isentropic efficiency exerts a positive effect on operational safety margin: the resulting increase in steam quality moves the system away from the critical limit $x \geq 0.88$, thereby reducing the risk of blade erosion. However, this apparent benefit should be interpreted with caution, since higher quality at the end of the expansion also implies greater heat rejection in the condenser and, consequently, lower global thermodynamic conversion efficiency. This trade-off underscores the importance of complementing the analysis with exergetic or thermoeconomic criteria to define truly optimal operating conditions.

5.3.7. Recommended Configuration

Based on multi-criteria analysis and its verification through sensitivity analysis, Configuration 1 is recommended for implementation in the Tula cogeneration system. This selection is founded on:

1. Superior operational flexibility: The operating range of 1365 bar·°C allows accommodating significant variations in HRSG conditions without requiring configuration changes. This flexibility is critical for adaptability to seasonal variations, changes in refinery load, or fluctuations in ambient conditions.
2. Performance–reliability balance: Configuration 1 generates 78.97 MW (97.7% of the absolute maximum) with an adequate safety margin (0.030) that protects against transient violations of steam quality. The sacrifice of 1.85 MW with respect to the absolute maximum is amply justified by greater operational robustness.
3. Competitive simplicity: Configuration 1 requires only 3 expansion stages, facilitating control and reducing maintenance costs. This simplicity also increases inherent system reliability by reducing potential failure points.
4. Acceptable robustness: The standard deviation of 2.20 MW (64% of best) provides sufficient thermodynamic consistency for operational planning. Although Configuration 2 presents lower variability, its restricted operating range severely limits its practical applicability.
5. Selection robustness: Sensitivity analysis confirms that Configuration 1 maintains superiority under different design philosophies, except in extreme scenarios that prioritize reliability over all other criteria.

For applications where absolute power maximization is prioritized (contexts with very high electricity prices or minimum generation contractual requirements), Configuration 3 could be justified provided that advanced monitoring and control systems are implemented to mitigate risks associated with operation near the steam quality limit ($\Delta x = 0.001$). However, such a scenario would require significant additional investments in instrumentation and protection systems.

Configuration 2, although presenting excellent reliability (best safety margin and lower variability), is not recommended for initial implementation due to its severely restricted operating range (462 bar·°C, only 34% of maximum). This configuration could be

considered in future applications with very specific and stable operating conditions within its narrow validity region.

5.4. Implementation Recommendations

Based on the multi-criteria evaluation of Section 5.4 and considering current operating conditions of the refinery, implementation of Configuration 1 is recommended with specifications presented in Table 14.

Table 14. Specifications of recommended design for initial implementation.

Parameter	Nominal Value	Operating Range
HRSG conditions		
Steam generation pressure	88–90 bar	75–140 bar
Superheat temperature	510 °C	500–520 °C
Active components		
Distribution headers	Head I, Head II	
Expansion valves	EV ₁ , EV ₂ , EV ₃	
Steam turbines	ST ₁ , ST ₃ , ST ₅	
Number of expansion stages	3	
Expected performance		
Steam cycle power	72.32 MW	68–79 MW
Total combined cycle power	360.90 MW	356–367 MW
Utilization factor	0.710	0.705–0.718
Specific fuel consumption	0.207 kg/kWh	0.204–0.210 kg/kWh
Improvement with respect to base system ^a		
Increment in total power	+72.32 MW	–
Improvement in utilization factor	+11.09 %	–
Reduction in SFC	–20.01 %	–

^a Improvement percentages will be calculated once base system performance is determined (gas turbines + conventional boilers).

The recommended operating range (75–140 bar, 500–520 °C, Table 6) accommodates exhaust gas variations across the four gas turbine trains without requiring reconfiguration of the active steam cycle topology. Dynamic analysis (start-up, load following, demand variation) is identified as future work.

This configuration provides optimal balance between the following attributes:

1. Increased generation: Produces 72.32 MW of additional power under nominal conditions.
2. Improved efficiency: Maintains utilization factor of 0.710, reaching typical values of state-of-the-art combined cycle plants.
3. Reduced consumption: Achieves specific consumption of 0.207 kg/kWh, decreasing operating costs and CO₂ emissions proportionally.
4. Operational flexibility: Offers wide operating range (75–140 bar in pressure, 500–520 °C in temperature), allowing adaptation to variations in steam demands or equipment availability.
5. Safety margin: Maintains distance of 0.030 from critical steam quality limit, sufficient for reliable operation under transient variations.
6. Moderate complexity: Requires only three expansion stages, facilitating operation, control, and system maintenance.

5.4.1. Incremental Optimization Strategies

If HRSG rehabilitation with improved specifications is contemplated, two strategies are identified that maintain Configuration 1 as the optimal topology.

Strategy A: Pressure Increase

Increase steam generation pressure to 130–140 bar while maintaining superheat temperature in the nominal range 510–520 °C.

Expected benefits:

- Power increment of 5–6 MW (reaching 77–79 MW);
- Improvement of 0.7% in utilization factor (reaching $UF = 0.716$ – 0.718);
- Additional reduction of 1.4% in specific fuel consumption (reaching $SFC = 0.204$ – 0.206 kg/kWh);
- Maintenance of adequate safety margin ($x_{\min} = 0.910$ – 0.915).

Technical requirements:

- HRSGs designed for operating pressure of 140 bar with appropriate safety margin (design pressure typically 1.2 times operating pressure);
- Modifications in the steam distribution system piping and valves to support increased pressure;
- Recertification of steam turbines for operation in new pressure range.

Strategy B: Nominal Point Optimization

Adjust nominal conditions within current HRSG range to approach thermodynamic optimum. Specifically, operate at ($P_{\text{HRSG}} = 88$ – 90 bar, $T_{s4} = 500$ °C) instead of original conditions at 510 °C.

Expected benefits:

- Increment of 1–2 MW (reaching 74–75 MW);
- Marginal improvement in utilization factor (0.3–0.5%);
- No additional capital investment requirements.

Additional considerations: Superheat temperature reduction could extend the service life of HRSG thermal components by operating under less severe conditions, potentially extending maintenance intervals.

The decision between these strategies must be founded on technical–economic analysis that quantifies incremental investment costs, additional revenues from higher electric generation, and savings in fuel consumption. This analysis must calculate the payback period and net present value under different scenarios of electricity and natural gas prices.

5.4.2. Future Expansion Scenario: Transition to Configuration 3

If future operating conditions justify maximization of electric generation at the expense of increased complexity and reduced safety margins, Configuration 3 represents viable expansion option. This transition is recommended only if the following conditions are met:

Condition 1: HRSG Modification

HRSGs must be modified to operate in the range $P_{\text{HRSG}} = 130$ – 140 bar and $T_{s4} = 550$ – 560 °C. This requires replacement or reinforcement of high-temperature components, particularly superheaters and connection piping. Additionally, combustion control system upgrade is required to maintain elevated temperatures with stability.

Condition 2: Complete ST_4 Installation

Turbine ST_4 must be installed with both operational expansion stages (HP → LP and LP → COND). This installation requires investment in multi-stage turbine with controlled extractions and regulation valve systems for each stage.

Condition 3: Advanced Monitoring Systems

Implement continuous monitoring of steam quality through humidity sensors at outlets of all turbine stages, particularly at ST₄ outlet where $x \approx 0.88$. The system must include anticipatory alarms and automatic interlock that reduces superheat temperature if quality approaches dangerously close to the limit.

Condition 4: Economic Justification

Additional investment must be justified through cost–benefit analysis demonstrating that incremental revenues from higher electric generation exceed increased investment, operation, and maintenance costs in an acceptable payback period. Expected power increment is approximately an additional 8 MW, equivalent to 4960 MWh/month, assuming a plant factor of 0.85. Typically, an acceptable payback period for industrial projects is less than 5 years.

Under these conditions, transition to Configuration 3 would generate the following results:

- Power of 80.82 MW (11% increase with respect to nominal Config. 1);
- Utilization factor of 0.735 (3.4% increase);
- Specific fuel consumption of 0.199 kg/kWh (3.9% reduction).

However, it would operate with minimum steam quality of 0.880, requiring rigorous operational management and advanced protection systems.

5.4.3. Applicability to Other PEMEX System Refineries

The methodology developed in this work is directly applicable to other refineries of the PEMEX system (Salamanca, Salina Cruz, Minatitlán, Cadereyta, Ciudad Madero) through the systematic procedure summarized in Table 15.

Table 15. Procedure for applying methodology to other refineries.

Step	Phase	Main Activities
1	Characterization	Identify specific steam demands (pressure levels, temperatures, mass flows). Characterize existing equipment (gas turbines, HRSGs if applicable, steam infrastructure).
2	Superstructure generation	Apply three-step procedure described in Section 3.3. Evaluate expansion viability through criterion $x \geq 0.88$. Define multi-stage turbines according to Table 5.
3	Parametric exploration	Determine relevant ranges of $(P_{\text{HRSG}}, T_{s_4})$ according to technological limitations. Implement MINLP model according to formulation of Section 4.3. Evaluate 80–100 parametric combinations.
4	Configuration identification	Construct optimal configuration map analogous to Table 10. Analyze mechanisms of transitions between configurations. Predict thresholds through thermodynamic analysis.
5	Multi-criteria evaluation	Adapt criteria from Table 12 to specific priorities. Perform weight sensitivity analysis. Recommend design considering particular restrictions.

This procedure is generalizable because it is founded on universal thermodynamic principles: mass and energy balances, steam quality restrictions, and MINLP optimization.

Particularities of each installation (pressure levels, temperatures, flows) are incorporated as input data to the model, without requiring reformulation of mathematical structure.

Quantification of aggregate improvement potential in the national refinery system requires detailed evaluation specific to each installation. Factors to consider include

- Availability of existing gas turbines or viability of new installation
- Current configuration of steam generation system (conventional boilers vs. existing HRSGs)
- Steam demand profiles at multiple pressure levels
- Physical space restrictions and connections with existing infrastructure
- Technical-economic feasibility considering investment costs and applicable regulatory framework

This aggregate evaluation constitutes relevant future work to inform national energy policy in the petroleum refining sector. Systematic implementation of advanced cogeneration in the refinery system presents significant potential for improvement in global energy efficiency.

6. Conclusions

This work demonstrates that the optimal topology of a cogeneration system does not vary continuously with design parameters but undergoes discrete transitions at specific thermodynamic thresholds. This finding challenges the conventional assumption in the optimization literature—which traditionally addresses parameter selection and topological configuration separately—and has fundamental implications for the design of flexible energy systems.

Through systematic parametric exploration (70–140 bar and 500–560 °C) coupled with superstructure-based MINLP optimization, three topologically distinct configurations that maximize power generation under different operating conditions were identified. The principal scientific contribution lies in the rigorous characterization of the mechanisms governing these transitions:

1. **Configuration 2 → 1 Transition (100–110 bar):** Occurs when HRSG pressure increases at constant temperature, raising the ST4 outlet temperature (T_{s13}) until the LP header mixing constraint ($T_{s13} < 350$ °C) activates, rendering Configuration 2 thermodynamically infeasible. The optimizer responds by activating valve EV3 for tempering with saturated steam (Configuration 1).
2. **Configuration 1 → 3 Transition (>530 °C):** Emerges from the trade-off between power maximization and steam quality degradation. At elevated temperatures, Configuration 1 develops excessive quality ($x_{s19} > 0.940$) with diminishing power output, while Configuration 3 divides the high-pressure expansion into two stages (ST4), generating an additional 4–8 MW while maintaining quality near the safety limit ($x_{s14} \approx 0.88$).

This mechanistic understanding fundamentally transforms design methodology: rather than discovering operational limitations through field-testing, engineers can now anticipate topology changes during the design phase by evaluating critical constraint activation across the entire anticipated operating envelope.

From a practical perspective, **Configuration 1** (active ST1 + ST3 + ST5, operational valves EV1–EV3) emerges as the recommended design for the Miguel Hidalgo refinery following multi-criteria evaluation integrating maximum power, operating range, safety margin, system simplicity, and performance robustness. With a weighted score of 0.82 (versus 0.69 and 0.68 for alternatives), this configuration offers

- **High performance:** 72.32 MW from the steam cycle under nominal conditions, representing a 25% increase in total generation (288 MW baseline + 72.32 MW additional).
- **Broad operational flexibility:** A valid range of 75–140 bar and 500–520 °C (1365 bar·°C), enabling adaptation to seasonal variations and demand changes without reconfiguration.
- **Adequate safety margin:** $\Delta x = 0.03$ above the critical quality limit ($x \geq 0.88$), protecting against blade erosion during transients.
- **Moderate complexity:** Only three expansion stages, facilitating control and maintenance.

In terms of energy efficiency, this translates to an 11.09% improvement in utilization factor (from 0.640 to 0.710) and a 20% reduction in specific fuel consumption (from 0.259 to 0.207 kg/kWh) relative to the baseline system without cogeneration. The additional annual generation (534 GWh, assuming an 85% plant factor) is equivalent to the residential consumption of approximately 160,000 Mexican households.

The developed methodology—systematized into a five-step procedure (characterization → superstructure generation → parametric exploration → configuration identification → multi-criteria evaluation)—is directly generalizable to other PEMEX refineries (Salamanca, Salina Cruz, Minatitlán, Cadereyta, Ciudad Madero) and to industrial installations worldwide. Preliminary estimates suggest an aggregate efficiency improvement potential of 15–25% across the refinery portfolio, translating to 400–600 GWh annually in additional electricity generation and proportional CO₂ emissions reductions.

Four priority directions emerge for future work: (1) systematic quantification of aggregate potential across the national refinery system to inform energy policy; (2) detailed exergy analysis to identify irreversibilities and targeted improvement opportunities; (3) extension to multi-objective optimization integrating economic (capital cost, payback period) and environmental (CO₂, NO_x emissions) variables; and (4) investigation of similar discrete transition phenomena in other industrial energy systems with multi-pressure steam networks.

The demonstration that optimal cogeneration system topology transitions discretely at thermodynamically explainable thresholds fundamentally alters how flexible energy systems should be designed. This work provides both theoretical understanding and practical tools enabling designers to anticipate configuration changes during the design phase, rather than discovering them through costly operational trial-and-error.

Author Contributions: Conceptualization, M.S.-P., L.E.M.-C., R.L.-L. and H.D.L.-M.; methodology, M.S.-P., L.E.M.-C. and H.D.L.-M.; software, M.S.-P., L.E.M.-C. and H.D.L.-M.; validation, M.S.-P. and R.L.-L.; formal analysis, R.L.-L., M.S.-P. and L.E.M.-C.; investigation, M.S.-P. and L.E.M.-C.; resources, M.S.-P., L.E.M.-C., W.B.-B., R.L.-L., S.C.-H. and H.D.L.-M.; data curation, M.S.-P., L.E.M.-C. and H.D.L.-M.; writing—original draft preparation, M.S.-P. and L.E.M.-C.; writing—review and editing, L.E.M.-C., R.L.-L., S.C.-H. and H.D.L.-M.; visualization, M.S.-P., R.L.-L. and H.D.L.-M.; supervision, M.S.-P. and H.D.L.-M.; project administration, M.S.-P. and W.B.-B. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

Nomenclature

Equipment Inventory of the Superstructure

HRSG System

EC	Economizer
EV	Evaporator
SH	Superheater
Drum	Liquid-Vapor Separator

Distribution Headers

Head I	Superheated Steam Header
Head II	Saturated Steam Header
Head HP	High-Pressure Header (Refinery Supply)
Head LP	Low-Pressure Header (Refinery Supply)

Bifurcation Nodes

Node 1	Bifurcation Node 1
Node 2	Bifurcation Node 2
Node 3	Bifurcation Node 3

Expansion Valves

EV ₁	Expansion Valve 1
EV ₂	Expansion Valve 2
EV ₃	Expansion Valve 3
EV ₄	Expansion Valve 4

Steam Turbines

ST ₁	Steam Turbine 1 (3 stages, with electric generator)
ST ₂	Steam Turbine 2 (3 stages, with electric generator)
ST ₃	Steam Turbine 3 (2 stages, with electric generator)
ST ₄	Steam Turbine 4 (2 stages, with electric generator)
ST ₅	Steam Turbine 5 (1 stage, with electric generator)
ST ₆	Steam Turbine 6 (1 stage)

Condensate System

COND	Condenser
P	Feedwater Pump
Tank	Water Makeup Tank

Symbols and Variables

Latin Letters

$c_{p,a}$	Specific heat capacity of air at constant pressure	$\text{kJ}/(\text{kg}\cdot\text{K})$
$c_{p,g}$	Specific heat capacity of gas at constant pressure	$\text{kJ}/(\text{kg}\cdot\text{K})$
h	Specific enthalpy	kJ/kg
h_{HP}	Specific enthalpy at high-pressure header	kJ/kg
h_{LP}	Specific enthalpy at low-pressure header	kJ/kg
j	Steam turbine number index	-
k	Expansion stage index	-
$\dot{m}$	Mass flow rate	kg/s
$\dot{m}_a$	Air mass flow rate	kg/s
$\dot{m}_f$	Fuel mass flow rate	kg/s
$\dot{m}_g$	Exhaust gas mass flow rate	kg/s
$\dot{m}_T$	Total steam mass flow rate	kg/s
$\dot{m}_{\text{HP}}$	High-pressure steam mass flow rate	kg/s
$\dot{m}_{\text{LP}}$	Low-pressure steam mass flow rate	kg/s
m	Inlet state index	-
$m + 1$	Outlet state index	-
P	Pressure	bar
P_0	Reference pressure	bar
P_{g1}	Gas turbine inlet pressure	bar

P_{g2}	Compressor outlet pressure	bar
P_{g3}	Turbine inlet pressure	bar
P_{g4}	Turbine outlet pressure	bar
P_{HRSG}	HRSG operating pressure	bar
$\dot{Q}$	Heat flow rate	MW
$\dot{Q}_{CC}$	Heat flow rate supplied to combustion chamber	MW
$\dot{Q}_{HP}$	High-pressure steam heat flow rate	MW
$\dot{Q}_{LP}$	Low-pressure steam heat flow rate	MW
T	Temperature	°C
T_0	Reference temperature	°C
T_{g1}	Gas turbine inlet temperature	°C
T_{g2}	Compressor outlet temperature	°C
T_{g3}	Turbine inlet temperature	°C
T_{g4}	Turbine outlet temperature	°C
T_{ge}	Gas temperature at evaporator outlet	°C
T_{sat}	Saturation temperature	°C
T_{s4}	Superheater outlet temperature	°C
$\dot{W}$	Power	MW
$\dot{W}_P$	Pump power consumption	MW
$\dot{W}_{m,ST}$	Steam cycle power output	MW
$\dot{W}_{m,TG}$	Gas turbine power output	MW
$\dot{W}_{m,CC}$	Combined cycle power output	MW
$\dot{W}_{ST_j}$	Power generated by steam turbine j	MW
$\dot{W}_{ST_1}$	Power generated by steam turbine 1	MW
$\dot{W}_{ST_2}$	Power generated by steam turbine 2	MW
$\dot{W}_{ST_3}$	Power generated by steam turbine 3	MW
$\dot{W}_{ST_4}$	Power generated by steam turbine 4	MW
$\dot{W}_{ST_5}$	Power generated by steam turbine 5	MW
$\dot{W}_{ST_6}$	Power generated by steam turbine 6	MW
y_{ST}	Binary variable for steam turbine expansion stages	-
$y_{ST_{jk}}$	Binary variable for expansion stage k of turbine j	-
z_i	Binary variable for steam flow i	-
Greek Letters		
γ	Specific heat ratio	-
γ_a	Specific heat ratio of air	-
γ_g	Specific heat ratio of exhaust gas	-
ΔP	Pressure drop	-
ΔP_{CC}	Pressure drop in combustion chamber	-
ΔP_{GT}	Pressure drop in gas turbine	-
ΔT_{PP}	Pinch Point temperature difference	°C
η	Efficiency	-
η_s	Isentropic efficiency	-
$\eta_{s,ST_{jk}}$	Isentropic efficiency of expansion stage k in turbine j	-
η_{sic}	Isentropic efficiency of compressor	-
η_{sit}	Isentropic efficiency of turbine	-
π_C	Compression ratio	-
Subscripts and Notation		
0	Reference state	
1, 2, 3, ..., 34	State points in the thermodynamic cycle	
a	Air	
CC	Combustion chamber	
f	Fuel	
g	Gas/exhaust gas	
$g1, g2, g3, g4$	Gas turbine cycle states	

<i>ge</i>	Gas at evaporator outlet
<i>HP</i>	High pressure
<i>HRSG</i>	Heat recovery steam generator
<i>i</i>	Flow index
<i>j</i>	Steam turbine number
<i>jk</i>	Expansion stage <i>k</i> of turbine <i>j</i>
<i>k</i>	Expansion stage
<i>LP</i>	Low pressure
<i>m</i>	Mechanical/output or inlet state
<i>m + 1</i>	Outlet state
<i>P</i>	Pump
<i>s</i>	Steam or isentropic
<i>s₄</i>	Superheater outlet state
<i>sat</i>	Saturation
<i>ST</i>	Steam turbine
<i>ST₁, ..., ST₆</i>	Steam turbines 1 through 6
<i>T</i>	Total
<i>TG</i>	Gas turbine

Appendix A. Thermodynamic States of the Superstructure

Table A1. Thermodynamic states of the Superstructure and mass flows for optimal configurations 1 and 2, for operating conditions of $P_{HRSG} = 88.26$ bar and $T_{s_4} = 510$ °C.

State	<i>P</i> (Bar)	<i>T</i> (°C)	<i>h</i> (kJ/kg)	<i>s</i> (kJ/kg K)	<i>x</i> (-)	Optimal Configuration <i>m_s</i> (kg/s)	
						1	2
<i>s₁</i>	88.26	42.76	186.82	0.6055	SCL	163.74	163.74
<i>s₂</i>	88.26	301.95	1355.73	3.2733	SL	163.74	163.74
<i>s₃</i>	88.26	301.95	2745.74	5.6902	DSS	163.74	163.74
<i>s₄</i>	88.26	510.00	3414.53	6.7035	SHS	105.83	163.74
<i>s₅</i>	88.26	510.00	3414.53	6.7035	SHS	45.73	4.32
<i>s₆</i>	60	450.27	3303.40	6.7225	SHS	45.73	4.32
<i>s₇</i>	20	303.23	3031.73	6.7815	SHS	0.00	0.00
<i>s₈</i>	0.0738	40.00	2213.09	7.1046	0.8502	0.00	0.00
<i>s₉</i>	88.26	510.00	3414.53	6.7035	SHS	60.10	159.42
<i>s₁₀</i>	60	496.46	3414.53	6.8715	SHS	60.10	159.42
<i>s₁₁</i>	60	496.46	3414.53	6.8715	SHS	0.00	9.57
<i>s₁₂</i>	60	496.46	3414.53	6.8715	SHS	0.00	98.22
<i>s₁₃</i>	20	342.50	3120.88	6.9312	SHS	0.00	98.22
<i>s₁₄</i>	0.0738	40.00	2264.61	7.2691	0.8716	0.00	0.00
<i>s₁₅</i>	60	496.46	3414.53	6.8715	SHS	60.10	51.62
<i>s₁₆</i>	20	475.69	3414.53	7.3631	SHS	60.10	51.62
<i>s₁₇</i>	20	475.69	3414.53	7.3631	SHS	14.42	5.94
<i>s₁₈</i>	20	475.69	3414.53	7.3631	SHS	45.68	45.68
<i>s₁₉</i>	0.0738	40.00	2417.28	7.7567	0.9351	45.68	45.68
<i>s₂₀</i>	88.26	301.95	2745.74	5.6902	DSS	57.91	0.00
<i>s₂₁</i>	88.26	301.95	2745.74	5.6902	DSS	0.00	0.00
<i>s₂₂</i>	60	275.59	2682.70	5.7044	0.9352	0.00	0.00
<i>s₂₃</i>	20	212.38	2511.38	5.7481	0.8481	0.00	0.00
<i>s₂₄</i>	0.0738	40.00	1867.82	6.0021	0.7067	0.00	0.00
<i>s₂₅</i>	88.26	301.95	2745.74	5.6902	DSS	57.91	0.00
<i>s₂₆</i>	60	275.59	2745.74	5.8193	0.9753	57.91	0.00
<i>s₂₇</i>	60	275.59	2745.74	5.8193	0.9753	57.91	0.00
<i>s₂₈</i>	60	275.59	2745.74	5.8193	0.9753	0.00	0.00
<i>s₂₉</i>	20	212.38	2745.74	6.2307	0.9721	0.00	0.00

Table A2. Continuation of thermodynamic states of the Superstructure and mass flows for optimal configurations 1 and 2, for operating conditions of $P_{HRSG} = 88.26$ bar and $T_{s4} = 510$ °C.

State	P (Bar)	T (°C)	h (kJ/kg)	s (kJ/kg K)	x (-)	Optimal Configuration $\dot{m}_s$ (kg/s)	
						1	2
s ₃₀	60	482.00	3380.00	6.8261	SHS	89.75	0.00
s ₃₁	20	330.16	3093.15	6.8857	SHS	89.75	0.00
s ₃₂	0.0738	40.00	2248.88	7.2189	0.8651	0.00	0.00
s ₃₃	20	350	3137.64	6.9582	SHS	0.00	0.00
s ₃₄	0.0738	40.00	2274.00	7.2991	0.8755	0.00	0.00
s ₃₅	0.0738	40.00	167.54	0.5724	SL	45.68	45.68
s _{HP}	60	482	3380.00	6.8261	SHS	13.89	13.89
s _{LP}	20	350	3137.64	6.9582	SHS	104.17	104.17

Table A3. Thermodynamic states of the Superstructure and mass flows for optimal configuration 3, for operating conditions of $P_{HRSG} = 88.26$ bar and $T_{s4} = 530$ °C.

State	P (Bar)	T (°C)	h (kJ/kg)	s (kJ/kg K)	x (-)	$\dot{m}_s$ (kg/s)
s ₁	88.26	42.76	186.82	0.6055	SCL	159.87
s ₂	88.26	301.95	1355.73	3.2733	SL	159.87
s ₃	88.26	301.95	2745.74	5.6902	DSS	159.87
s ₄	88.26	530.00	3464.31	6.7662	SHS	104.66
s ₅	88.26	530.00	3464.31	6.7662	SHS	44.35
s ₆	60	469.30	3349.50	6.7854	SHS	44.35
s ₇	20	319.35	3068.68	6.8448	SHS	0
s ₈	0.0738	40.00	2234.78	7.1739	0.8592	0
s ₉	88.26	530.00	3464.31	6.7662	SHS	60.31
s ₁₀	60	517.43	3464.31	6.9353	SHS	60.31
s ₁₁	60	517.43	3464.31	6.9353	SHS	0
s ₁₂	60	517.43	3464.31	6.9353	SHS	49.17
s ₁₃	20	360.45	3160.90	6.9953	SHS	7.36
s ₁₄	0.0738	40.00	2286.87	7.3402	0.8809	41.81
s ₁₅	60	517.43	3464.31	6.9353	SHS	11.14
s ₁₆	20	498.28	3464.31	7.4286	SHS	11.14
s ₁₇	20	498.28	3464.31	7.4286	SHS	11.14
s ₁₈	20	498.28	3464.31	7.4286	SHS	0
s ₁₉	0.0738	40.00	2441.01	7.8325	0.9449	0

Table A4. Continuation of thermodynamic states of the Superstructure and mass flows for optimal configuration 3, for operating conditions of $P_{HRSG} = 88.26$ bar and $T_{s4} = 530$ °C.

State	P (Bar)	T (°C)	h (kJ/kg)	s (kJ/kg K)	x (-)	$\dot{m}_s$ (kg/s)
s ₂₀	88.26	301.95	2745.74	5.6902	DSS	55.21
s ₂₁	88.26	301.95	2745.74	5.6902	DSS	0
s ₂₂	60	275.59	2682.70	5.7044	0.9352	0
s ₂₃	20	212.38	2511.38	5.7481	0.8481	0
s ₂₄	0.0738	40.00	1867.82	6.0021	0.7067	0
s ₂₅	88.26	301.95	2745.74	5.6902	DSS	55.21
s ₂₆	60	275.59	2745.74	5.8193	0.9753	55.21
s ₂₇	60	275.59	2745.74	5.8193	0.9753	55.21
s ₂₈	60	275.59	2745.74	5.8193	0.9753	0
s ₂₉	20	212.38	2745.74	6.2307	0.9721	0
s ₃₀	60	482.00	3380.00	6.8261	SHS	85.67
s ₃₁	20	330.16	3093.15	6.8857	SHS	85.67
s ₃₂	0.0738	40.00	2248.88	7.2189	0.8651	0
s ₃₃	20	350.00	3137.64	6.9582	SHS	0
s ₃₄	0.0738	40.00	2274.00	7.2991	0.8755	0
s ₃₅	0.0738	40.00	167.54	0.5724	SL	41.81
s _{HP}	60	482.00	3380.00	6.8261	SHS	13.89
s _{LP}	20	350.00	3137.64	6.9582	SHS	104.17

Appendix B. Computational Implementation Details

This appendix provides comprehensive specifications of the computational environment, numerical methods, and implementation procedures used throughout this work, enabling exact replication of results presented in Section 5.

Appendix B.1. Software Environment

The optimization framework was implemented in Microsoft Excel 2019 (Version 16.0.10396) with the following components:

- Solver Engine: GRG (Generalized Reduced Gradient) Nonlinear solver, part of Excel Solver Add-in developed by Frontline Systems
- Thermodynamic Properties: XSteam add-in version 2.6 (Magnus Holmgren, 2006), implementing IAPWS-IF97 formulas for water and steam properties
- Operating System: Windows 10 Professional (64-bit)
- Hardware: Intel Core i7-9700 processor (3.0 GHz, 8 cores), 16 GB RAM

Alternative implementations are feasible in any environment supporting MINLP solvers and IAPWS-IF97 property calculations, including:

- Python --> 3.10 with `scipy.optimize` + `iapws` library
- Julia --> 1.11.0 with `JuMP.jl` + `Juniper.jl` + `IAPWS.jl`
- Gams --> 40.1.0 with BARON or DICOPT solvers

Appendix B.2. Complete Solver Configuration

The GRG Nonlinear solver was configured with the following parameters to ensure robust convergence:

Parameter	Value	Purpose
Convergence tolerance	10^{-6}	Gradient norm threshold
Constraint precision	10^{-5}	Feasibility tolerance
Maximum iterations	1000	Prevents infinite loops
Maximum subproblem iterations	500	Per NLP subproblem
Derivatives method	Forward difference	Numerical gradients
Central differences	Enabled	Improved accuracy
Multistart	10 runs	Escape local optima
Population size	50	Initial point generation
Random seed	Variable	Different for each case

These settings balance computational efficiency (typical solution time 2–5 min per case) with solution quality. Tighter tolerances (10^{-8}) were tested but provided negligible improvement at $3\text{--}5\times$ computational cost.

Appendix B.3. Solution Algorithm

The complete solution procedure for each parametric case (P_{HRSG}, T_{s_4}) follows this structured methodology:

Algorithm: MINLP Solution for Single Operating Point

Input: (P_{HRSG}, T_{s_4}), refinery demands ($\dot{m}_{\text{HP}}, \dot{m}_{\text{LP}}$)

Output: Optimal configuration, power $\dot{W}_{\text{net}}$, state points

Step 1: Calculate HRSG steam generation

1. Evaluate gas turbine cycle using Equations (3)–(6)
2. Calculate $\dot{m}_T$ from HRSG energy balance with pinch point constraint (Equation (8))

3. Verify stack temperature $T_{g7} \geq 120$ °C to avoid acid condensation

Step 2: Identify candidate configurations

Based on systematic thermodynamic feasibility analysis of the superstructure (Section 3), three topologically distinct configurations identified as optimal in adjacent parametric regions are considered:

4. Configuration 1 (Tempering via Valves):

- Active Headers: Head I, Head II
- Active valves: EV_1 , EV_2 , EV_3
- Active turbines: ST_1 (3 stages), ST_3 (2 stages), ST_5 (1 stage)
- Fixed binary variables:
 - Set $y_{ST_1} = [1, 1, 1]$ (heuristic: activate ST_1 fully based on the highest enthalpy drop)
 - Set $y_{ST_3} = [1, 1, 0]$ (activate two stages)
 - Set $y_{ST_5} = [1]$ (activate single stage to condenser)
 - Set all other $y_{jk} = 0$ (remaining turbines and stages inactive)
 - Set $EV_1 = 1$, $EV_2 = 1$ and $EV_3 = 1$

5. Configuration 2 (Simplified System):

- Active Headers: Head I only (Head II deactivated)
- Active valves: EV_1 and EV_2 (EV_3 deactivated)
- Active turbines: ST_1 (3 stages), ST_4 (2 stages), ST_5 (1 stage)
 - Set $y_{ST_1} = [1, 1, 1]$ (heuristic: activate ST_1 fully based on the highest enthalpy drop)
 - Set $y_{ST_4} = [1, 1, 0]$ (activate two stages)
 - Set $y_{ST_5} = [1]$ (activate single stage to condenser)
 - Set all other $y_{jk} = 0$ (remaining turbines and stages inactive)
 - Set $EV_1 = 1$ and $EV_2 = 1$

6. Configuration 3 (High-Power Multi-Stage):

- Active Headers: Head I and Head II
- Active valves: EV_1 , EV_2 and EV_3
- Active turbines: ST_1 (3 stages), ST_3 (2 stages), ST_4 (2 stage)
 - Set $y_{ST_1} = [1, 1, 1]$ (heuristic: activate ST_1 fully based on the highest enthalpy drop)
 - Set $y_{ST_3} = [1, 1, 0]$ (activate two stages)
 - Set $y_{ST_4} = [1, 1]$ (activate two stages to condenser)
 - Set all other $y_{jk} = 0$ (remaining turbines and stages inactive)
 - Set $EV_1 = 1$, $EV_2 = 1$ and $EV_3 = 1$
- Total expansion stages: 4
- Key characteristic: Maximizes expansion stages for higher power generation

Justification of Configuration Selection

- Steam quality constraints ($x \geq 0.88$ at all turbine outlets)
- Temperature requirements of high- and low-pressure headers ($T_{HP} = 482$ °C, $T_{LP} = 350$ °C)
- Pressure hierarchy feasibility ($P_{HRSG} > P_{HP} > P_{LP} > P_{COND}$)
- Thermodynamic feasibility of tempering routes
- Preliminary sensitivity analysis that identified discrete transition phenomena

Alternative configurations (e.g., ST_2 , ST_6 , different valve combinations) were preliminarily evaluated but were excluded because:

- Violation of steam quality constraints within the operating range
- Lower power generation compared to the three candidates
- Thermodynamic infeasibility (inability to meet temperature specifications)

Step 3: Solve NLP for each candidate configuration

For each configuration $k \in \{1, 2, 3\}$

- Fix binary variables to the values specified in Step 2 for configuration k : $y = y_{k, \text{fixed}}$
- Formulate NLP problem with only continuous variables:
 - maximize $f(x_{\text{cont}}, y_{k, \text{fixed}}) = \dot{W}_{\text{ST}}(x_{\text{cont}}, y_{k, \text{fixed}})$
 - subject to $g(x_{\text{cont}}, y_{k, \text{fixed}}) \leq 0$ where:
 - x_{cont} = continuous variables (mass flows, pressures, temperatures, etc.)
 - $y_{k, \text{fixed}}$ = binary variables FIXED to configuration k values
 - $g(\cdot)$ = constraints (mass balances, energy balances, $x \geq 0.88$, etc.)
- Initialize continuous variables using heuristics:
 - Mass flows proportional to turbine enthalpy drops
 - Extraction pressures at demand levels ($P_{\text{HP}} = 60$ bar, $P_{\text{LP}} = 20$ bar)
 - Temperatures from isentropic expansion estimates with $\eta_{\text{IST}} = 0.89$
- Solve NLP using GRG Nonlinear with multistart strategy:
 - For $i = 1$ to 10 (multistart runs for continuous variables):
 - Generate random perturbation of initial continuous variables ($\pm 10\%$ variation)
 - Solve NLP from perturbed starting point
 - If solution is feasible and improves objective: Store solution
 - Select best solution among the 10 runs: $(x_{\text{cont}, k}^*, y_{k, \text{fixed}}, \dot{W}_k^*)$
- Verify thermodynamic consistency:
 - Mass balance closure: $|\sum \dot{m}_{\text{in}} - \sum \dot{m}_{\text{out}}| < 10^{-4}$ kg/s
 - Energy balance closure: $|\sum \dot{Q}_{\text{in}} - \sum \dot{Q}_{\text{out}} - \sum \dot{W}| / \sum \dot{Q}_{\text{in}} < 0.1\%$
 - Steam quality: $x_{jk} \geq 0.88$ at all active turbine stages
 - Entropy generation: $\dot{S}_{\text{gen}} \geq 0$ for all irreversible processes
- Thermodynamic feasibility check
 - If configuration k is thermodynamically feasible: Store $(x_{\text{cont}, k}^*, y_{k, \text{fixed}}, \dot{W}_k^*)$
 - If configuration k violates any constraint: Mark as infeasible for this point $(P_{\text{HRSG}}, T_{s4})$

Step 4: Multistart MINLP optimization

- Among feasible configurations, identify the one with maximum power: $k^* = \arg \max_{k \in \{1, 2, 3\}} \dot{W}_k^*$: configuration k is feasible
- Return optimal solution for this parametric point:
 - Configuration: k^*
 - Binary variables: $y_{k^*, \text{fixed}}$
 - Continuous variables: x_{cont, k^*}^*
 - Generated power: $\dot{W}_{k^*}^*$
 - All thermodynamic state points

Appendix B.4. Parametric Sweep Implementation

The complete parametric analysis evaluates 84–105 operating points depending on temperature range:

- Pressure sweep: $P_{\text{HRSG}} = [70, 75, 88.26, 90, 100, 110, 120, 130, 140]$ bar (9 values)
- Temperature sweeps:

- Low range: $T_{s_4} = [500, 510, 520] \text{ }^\circ\text{C} \rightarrow 9 \times 3 = 27$ cases
- Mid range: $T_{s_4} = [530, 540] \text{ }^\circ\text{C} \rightarrow 9 \times 2 = 18$ cases
- High range: $T_{s_4} = [550, 560] \text{ }^\circ\text{C} \rightarrow 9 \times 2 = 18$ cases
- Nominal case: (88.26 bar, 510 $^\circ\text{C}$) $\rightarrow 1$ case
- Total: $27 + 18 + 18 + \text{additional validation points} \approx 84\text{--}105$ cases

Each case requires 2–5 min solution time, totaling 7–9 h for a complete parametric map on the specified hardware. Parallel execution across multiple Excel instances can reduce wall-clock time proportionally to available cores (up to 8-fold speed upon the test system).

Appendix B.5. Three-Level Validation Protocol

All solutions undergo three-level validation before inclusion in results:

Level 1: Thermodynamic Consistency

- Energy balance closure: $|\sum \dot{Q}_{\text{in}} - \sum \dot{Q}_{\text{out}} - \sum \dot{W}| / \sum \dot{Q}_{\text{in}} < 0.1\%$
- Mass balance closure: $|\sum \dot{m}_{\text{in}} - \sum \dot{m}_{\text{out}}| < 10^{-3} \text{ kg/s}$ for each component
- Entropy generation: $\dot{S}_{\text{gen}} \geq 0$ for all irreversible processes (turbines, throttling valves, mixing)

Level 2: Physical Feasibility

- Steam quality: $x_{jk} \geq 0.88$ at all turbine stage outlets (safety criterion to prevent blade erosion)
- Temperature constraints: $T_{g7} \geq 120 \text{ }^\circ\text{C}$ (avoid sulfuric acid condensation in the stack)
- Pressure hierarchy: $P_{\text{HRSG}} > P_{\text{HP}} > P_{\text{LP}} > P_{\text{COND}}$ (ensure thermodynamic viability of flows)
- Flow positivity: $\dot{m}_i \geq 0$ for all streams (no negative or reverse flows)

Level 3: Solution Quality

- Convergence achieved: Gradient norm $< 10^{-6}$ (optimizer successfully found a stationary point)
- No binding constraints at tolerance: $|g_i| > 10^{-4}$ for active constraints (avoid numerical artifacts)
- Consistency across restarts: Best solutions from ≥ 3 random initializations agree within 0.1% (confirms robustness)

Cases failing any validation criterion are flagged for manual review. In this study, 98.7% of cases (83/84) passed all validation checks on the first attempt, with the single failure resulting from an infeasible pressure-temperature combination outside the steam tables' valid range.

Appendix B.6. Input Data Specification

Complete specification of input parameters, ensuring reproducibility:

Natural gas composition (volumetric basis):

- Methane (CH_4): 88.0% (primary component)
- Ethane (C_2H_6): 10.0%
- Propane (C_3H_8): 2.0%
- Trace components (N_2 , CO_2): $< 0.1\%$ (neglected in calculations)

Derived fuel properties:

- Lower heating value: $LHV = 49,514 \text{ kJ/kg}$ (calculated from composition using standard formation enthalpies)
- Molecular weight: $M_f = 17.63 \text{ kg/kmol}$
- Stoichiometric air-fuel ratio: $(A/F)_{\text{stoich}} = 16.12 \text{ kg}_{\text{air}}/\text{kg}_{\text{fuel}}$

- Actual air-fuel ratio: $(A/F)_{\text{actual}} = 42.25 \text{ kg}_{\text{air}}/\text{kg}_{\text{fuel}}$ (corresponds to 161.9% excess air, typical for industrial gas turbines)

Reference environment (Morris-Szargut method):

- Ambient temperature: $T_0 = 30 \text{ }^\circ\text{C}$ (303.15 K)—representative of Tula refinery location
- Ambient pressure: $P_0 = 0.78 \text{ bar}$ (Tula altitude: 2020 m above sea level)
- Reference state: Saturated liquid water at T_0 , P_0
- Dead state enthalpy: $h_0 = 125.74 \text{ kJ/kg}$
- Dead state entropy: $s_0 = 0.4365 \text{ kJ/(kg}\cdot\text{K)}$

These reference conditions are essential for calculating the utilization factor and comparing results with literature values, which often employ different reference states (25 °C, 1 bar being a common alternative).

References

1. Variny, M.; Jediná, D.; Kizek, J.; Illés, P.; Lukáč, L.; Janošovský, J.; Lesný, M. An investigation of the techno-economic and environmental aspects of process heat source change in a refinery. *Processes* **2019**, *7*, 776. [\[CrossRef\]](#)
2. Kornienko, V.; Radchenko, M.; Radchenko, A.; Koshlak, H.; Radchenko, R. Enhancing the Fuel Efficiency of Cogeneration Plants by Fuel Oil Afterburning in Exhaust Gas before Boilers. *Energies* **2023**, *16*, 6743. [\[CrossRef\]](#)
3. Costea, M.; Feidt, M. A Review Regarding Combined Heat and Power Production and Extensions: Thermodynamic Modelling and Environmental Impact. *Energies* **2022**, *15*, 8782. [\[CrossRef\]](#)
4. Mehrpooya, M.; Ashouri, M.; Mohammadi, A. Thermoeconomic analysis and optimization of a regenerative two-stage organic Rankine cycle coupled with liquefied natural gas and solar energy. *Energy* **2017**, *126*, 899–914. [\[CrossRef\]](#)
5. Pinto, L.F.R.; Tucci, H.N.P.; Mummolo, G.; Neto, G.C.d.O.; Facchini, F. Circular economy approach on energy cogeneration in petroleum refining. *Energies* **2022**, *15*, 1713. [\[CrossRef\]](#)
6. Chen, C.L.; Lin, C.Y. Design and optimization of steam distribution systems for steam power plants. *Ind. Eng. Chem. Res.* **2011**, *50*, 8097–8109. [\[CrossRef\]](#)
7. Golmohamadi, H.; Asadi, A. Integration of joint power-heat flexibility of oil refinery industries to uncertain energy markets. *Energies* **2020**, *13*, 4874. [\[CrossRef\]](#)
8. Ahmadi, P.; Dincer, I. Thermodynamic and exergoenvironmental analyses, and multi-objective optimization of a gas turbine power plant. *Appl. Therm. Eng.* **2011**, *31*, 2529–2540. [\[CrossRef\]](#)
9. Manesh, M.K.; Ghalami, H.; Amidpour, M.; Hamed, M. Optimal coupling of site utility steam network with MED-RO desalination through total site analysis and exergoeconomic optimization. *Desalination* **2013**, *316*, 42–52. [\[CrossRef\]](#)
10. Pariasamy, S.G.; Venkiteswaran, V.K.; Kumar, J.; Awad, M.M. Industrial CHP with steam systems: A review of recent case studies, trends and relevance to Malaysian industry. *Energies* **2022**, *15*, 7491. [\[CrossRef\]](#)
11. Lazzaretto, A.; Tsatsaronis, G. SPECO: A systematic and general methodology for calculating efficiencies and costs in thermal systems. *Energy* **2006**, *31*, 1257–1289. [\[CrossRef\]](#)
12. Toffolo, A.; Lazzaretto, A. Evolutionary algorithms for multi-objective energetic and economic optimization in thermal system design. *Energy* **2002**, *27*, 549–567. [\[CrossRef\]](#)
13. Bernier, E.; Maréchal, F.; Samson, R. Multi-objective design optimization of a natural gas-combined cycle with carbon dioxide capture in a life cycle perspective. *Energy* **2010**, *35*, 1121–1128. [\[CrossRef\]](#)
14. Bamufleh, H.S.; Ponce-Ortega, J.M.; El-Halwagi, M.M. Multi-objective optimization of process cogeneration systems with economic, environmental, and social tradeoffs. *Clean Technol. Environ. Policy* **2013**, *15*, 185–197. [\[CrossRef\]](#)
15. Grossmann, I.E.; Sargent, R.W. Optimum design of chemical plants with uncertain parameters. *AIChE J.* **1978**, *24*, 1021–1028. [\[CrossRef\]](#)
16. Li, J.; Demirel, S.E.; Hasan, M.F. Fuel gas network synthesis using block superstructure. *Processes* **2018**, *6*, 23. [\[CrossRef\]](#)
17. Variny, M.; Hanus, K.; Blahušák, M.; Furda, P.; Illés, P.; Janošovský, J. Energy and environmental assessment of steam management optimization in an ethylene plant. *Int. J. Environ. Res. Public Health* **2021**, *18*, 12267. [\[CrossRef\]](#)
18. Martelli, E.; Capra, F.; Consonni, S. Numerical optimization of combined heat and power organic Rankine cycles—part a: Design optimization. *Energy* **2015**, *90*, 310–328. [\[CrossRef\]](#)
19. Marty, F.; Serra, S.; Sochard, S.; Reneaume, J.M. Exergy analysis and optimization of a combined heat and power geothermal plant. *Energies* **2019**, *12*, 1175. [\[CrossRef\]](#)
20. Kemp, I.C.; Lim, J.S. *Pinch Analysis for Energy and Carbon Footprint Reduction: User Guide to Process Integration for the Efficient Use of Energy*; Butterworth-Heinemann: Oxford, UK, 2020.
21. Bejan, A.; Tsatsaronis, G.; Moran, M.J. *Thermal Design and Optimization*; John Wiley & Sons: New York, NY, USA, 1995.

22. Cotton, K.C. *Evaluating and Improving Steam Turbine Performance: Includes Cogeneration and Combined Cycles*; Cotton Fact Incorporated: Cary, NC, USA, 1998.
23. Tuma, M.; Oman, J.; Sekavčnik, M. Efficiency of a combined gas-steam process. *Energy Convers. Manag.* **1999**, *40*, 1163–1175. [[CrossRef](#)]
24. Albahri, T.A.; Khor, C.S.; Elsholkami, M.; Elkamel, A. A mixed integer nonlinear programming approach for petroleum refinery topology optimisation. *Chem. Eng. Res. Des.* **2019**, *143*, 24–35. [[CrossRef](#)]
25. Khor, C.; Elkamel, A. Superstructure optimization for oil refinery design. *Pet. Sci. Technol.* **2010**, *28*, 1457–1465. [[CrossRef](#)]
26. Kermani, M.; Wallerand, A.S.; Kantor, I.D.; Maréchal, F. Generic superstructure synthesis of organic Rankine cycles for waste heat recovery in industrial processes. *Appl. Energy* **2018**, *212*, 1203–1225. [[CrossRef](#)]
27. Masoumi, M.E.; Jahantighy, Z.F. Hydrogen Integration in Refinery Using MINLP Method. *Adv. Mater. Res.* **2013**, *622*, 720–725. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.