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An Open, Validated Design and Performance-Prediction Methodology for Ammonia Water Kalina-Cycle Recovery of Sub-150 °C Industrial Waste Heat

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Abstract

This study develops an open, verification-centered design and performance-prediction methodology for recovering sub-150 °C industrial waste heat with ammonia–water Kalina-cycle systems. The methodology is deliberately separated into source characterization, ammonia–water property verification, component-level mass/energy/exergy modeling, constrained cycle design, multi-variable optimization, surrogate performance prediction, uncertainty propagation, and reproducibility controls. The framework is motivated by the large but thermodynamically difficult inventory of low-temperature industrial heat and by the temperature-glide advantage of non-azeotropic ammonia–water working fluids. A reference implementation is defined around a configurable KCS-11-like architecture and an open workflow in which a process simulator such as DWSIM may host the flowsheet while Python-based scripts execute validation tests, optimization, surrogate fitting, and audit-ready reporting. A literature-anchored transparent reduced-order model is used only to demonstrate the workflow; it is not represented as a replacement for a validated ammonia–water equation of state. A 2,400-point synthetic design space spanning 80–150 °C source temperature, 0.55–0.95 ammonia mass fraction, 1.5–5.0 MPa high-side pressure, 3–10 K pinch, component efficiencies, sink temperature, recuperator effectiveness, and source duty is evaluated. The demonstration reproduces three published low-temperature benchmark efficiencies with a mean relative discrepancy of 2.73%, and a random-forest surrogate predicts the transparent model's net power with R^2 = 0.9825 and RMSE = 15.3 kW. Optimization shows that the best ammonia concentration and high-side pressure move with source temperature rather than remaining universal constants. Monte Carlo propagation further shows why design output should be reported as an uncertainty distribution rather than a single deterministic value. The principal contribution is therefore not a new proprietary Kalina correlation, but a transparent validation hierarchy and reproducible design protocol that can be implemented with qualified thermodynamic property routines and then extended to industrial project data.

KEYWORDS

Kalina Cycle; Ammonia–Water; Industrial Waste Heat; Low-Temperature Heat Recovery; KCS-11; Thermodynamic Validation; Exergy Analysis; Surrogate Modeling; Open-Source Process Simulation;

INTRODUCTION

Industrial waste heat is abundant but uneven in temperature, flow, composition, cleanliness, and temporal stability. A substantial share occurs at temperatures too low for conventional steam power generation to be attractive, even though the aggregate energy opportunity is large. The U.S. Department of Energy assessment by Johnson et al. (2008) documented large recoverable waste-heat streams across energy-intensive manufacturing and emphasized that technical opportunity depends not only on heat quantity but also on temperature and practical recovery constraints. Matsuda (2013) similarly identified waste heat below approximately 150 °C as a widely discarded industrial resource and described a low-heat power-generation implementation around a roughly 120 °C refinery overhead stream. These conditions define the central design problem addressed here: how to convert finite-capacity, sub-150 °C heat into electricity without overstating performance or hiding the thermodynamic assumptions that control the answer.

The Kalina cycle is one response to that problem. Kalina (1984) proposed a multicomponent working-fluid bottoming cycle in which mixture phase behavior can improve temperature matching between a sensible heat source and the working fluid. The ammonia–water pair is especially important because its composition can be adjusted and its phase change is non-isothermal. This temperature glide can reduce heat-transfer irreversibility when the mixture profile is well matched to the source, although the advantage is configuration- and boundary-condition-dependent rather than universal. The review by Zhang et al. (2012) shows that Kalina-cycle performance depends on architecture, mixture-property representation, ammonia concentration, pressure level, heat-source/sink temperatures, and practical concerns including safety and corrosion.

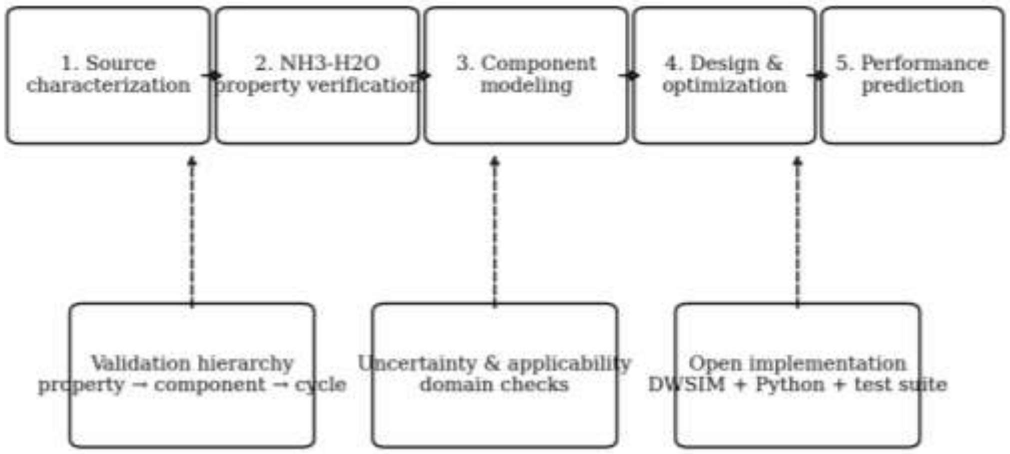
Low-temperature KCS-11 research provides a direct foundation for the present scope. Golubovic et al. (2007) examined KCS-11 performance for low-temperature heat sources and showed the strong influence of ammonia fraction and turbine inlet pressure. Ogriseck (2009) analyzed integration into a combined heat-and-power plant where flue gas was cooled from roughly 150 to 130 °C and reported net efficiency between 12.3% and 17.1% for the studied configuration and cooling conditions. These values should not be generalized to every sub-150 °C source, but they demonstrate that real integration decisions are governed by source/sink matching and working-fluid composition rather than source temperature alone.

A second challenge is reproducibility. Kalina-cycle calculations are sensitive to ammonia–water vapor–liquid equilibrium and enthalpy predictions. Tillner-Roth and Friend (1998a) systematically assessed available thermodynamic measurements, and Tillner-Roth and Friend (1998b) developed a Helmholtz-free-energy formulation valid over a broad thermodynamic domain, reporting reference uncertainties for VLE composition, density, and enthalpy. A credible open workflow therefore cannot simply state that a generic “property package” was used. It must identify the thermodynamic model, document its parameters and range, and prove that the selected implementation reproduces accepted reference behavior at the states traversed by the cycle.

The third challenge is computational. Design optimization across heat-source temperature, ammonia concentration, pressure, pinch constraints, recuperation, turbine efficiency, and cooling conditions can require thousands of nonlinear flash and heat-exchanger evaluations. Recent research has shown that data-driven surrogates can accelerate ammonia–water cycle analysis, but unconstrained black-box prediction can violate thermodynamic laws. Chen and Yuan (2023) demonstrated an ANN surrogate for an ammonia–water power cycle and showed that embedding thermal relations can improve generalization, particularly with limited data. Chen et al. (2025) extended this direction with thermodynamics-consistent machine learning and demonstrated the value of hard/soft constraints and anomaly handling. These developments motivate a methodology in which machine learning is subordinate to a verified thermodynamic solver rather than a replacement for it.

This article therefore develops an open design and performance-prediction methodology centered on verification, validation, applicability-domain control, and reproducibility. The paper does not claim new experimental Kalina-cycle measurements. Instead, it combines established literature, reference thermodynamic-property work, transparent governing equations, a literature-anchored reduced-order demonstration, and an open implementation architecture. The numerical figures reported in the results section are generated by the transparent demonstration model and are explicitly labeled as synthetic or illustrative wherever appropriate.

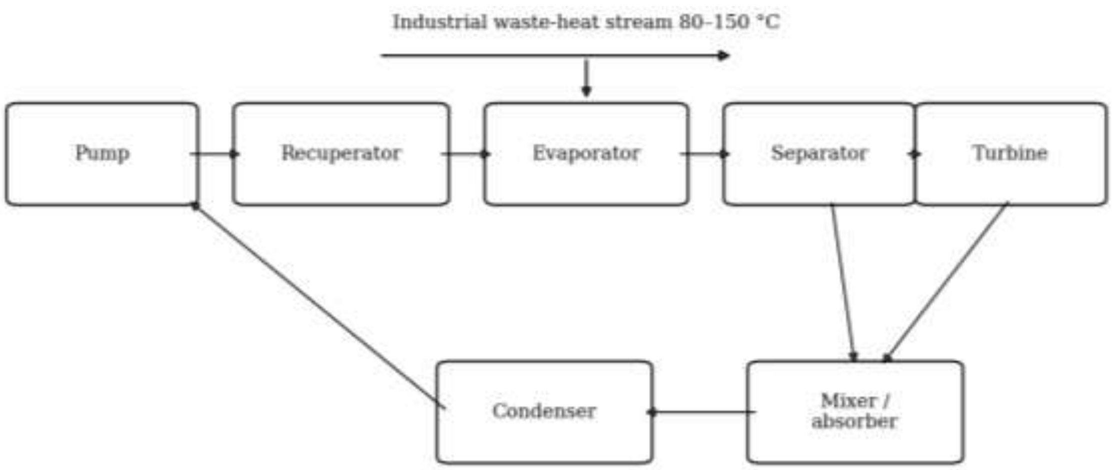
Figure 1: Open Validation-Centered Methodology for Sub-150 °C Kalina-Cycle Design



Background and Problem Statement

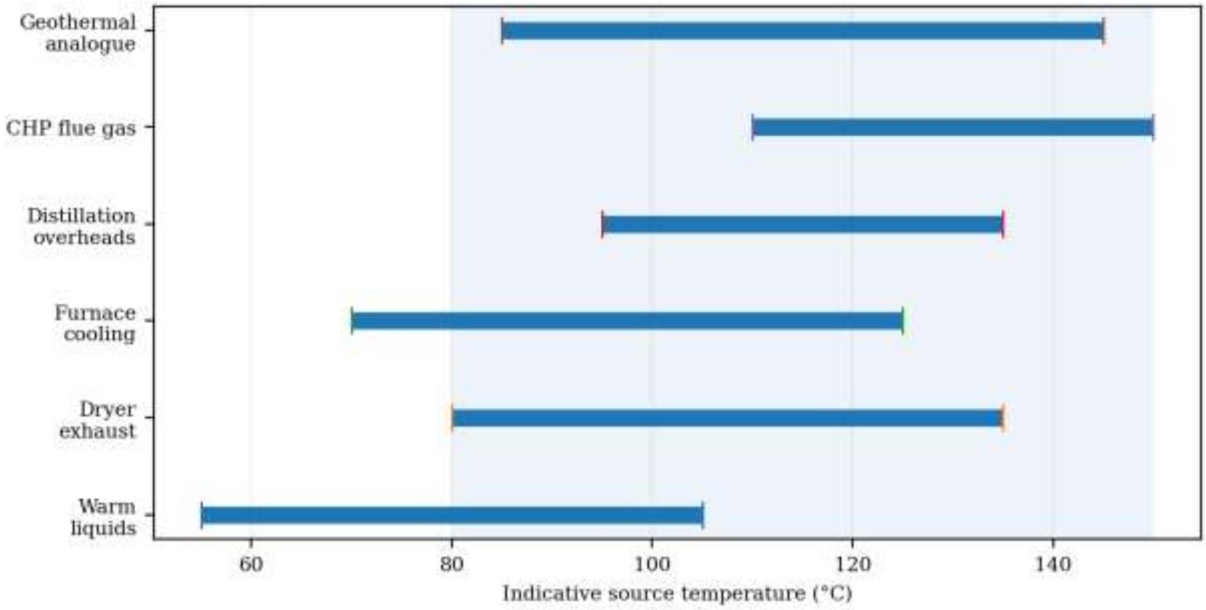
A sub-150 °C heat source is thermodynamically valuable but exergy-limited. Even before component losses are considered, the maximum work fraction falls as the source temperature approaches the heat sink. The engineering objective is consequently not to maximize thermal efficiency in isolation. A useful design must simultaneously recover a substantial fraction of the available heat, maintain feasible exchanger approach temperatures, avoid excessive ammonia circulation or pressure, preserve turbine expansion quality, satisfy material and safety requirements, and produce enough net power to justify the added equipment.

Figure 2: Configurable KCS-11-Like Ammonia–Water Recovery Architecture



The literature also shows that "optimal ammonia concentration" is not a single constant. Intakham et al. (2025) evaluated basic Kalina-cycle behavior over 100–150 °C and 1–7 MPa and found that the concentration associated with peak efficiency changes with pressure and evaporation temperature. Likewise, off-design analysis by Li et al. (2016) demonstrated that source temperature, source flow, and heat-sink temperature alter power output and control requirements. An open methodology must therefore produce operating envelopes and response surfaces, not merely one design point(Debasish, 2021; Md. Abdur & Iftekhar, 2021). Validation is the central unresolved problem addressed by this article. Many cycle papers report optimized efficiencies without making the full chain of property validation, mass/energy closure, pinch enforcement, benchmark comparison, numerical convergence, and uncertainty quantification equally visible (Debasish, 2022; Md Ashfaq & Abdullah Mohammad, 2022; Md Asif Ali Sheak & Risha, 2022). That approach makes replication difficult and can obscure whether disagreements arise from cycle architecture or from thermodynamic-property differences. The present framework responds by making validation hierarchical and explicit (Md. Rashedul & Md Kaium, 2022; Mohammad Abir Chowdhury & Tonay, 2022; Mohammad Shoriful Hossan, 2022).

Figure 3: Industrial and Analogous Low-Temperature Heat-Source Envelope



Purpose and Objectives of the Study

The purpose of the study is to formulate a transparent, open, and testable workflow for the preliminary design and performance prediction of ammonia–water Kalina systems driven by industrial waste heat below 150 °C . The objective is methodological rather than proprietary: each modeling layer should be independently testable, every performance output should be traceable to a property model and a set of boundary conditions, and surrogate predictions should remain inside a documented applicability domain. The specific objectives are to: (1) define a reproducible source-characterization protocol; (2) establish ammonia–water property verification as a prerequisite to cycle optimization; (3) formulate mass, species, energy, and exergy balances for a KCS-11-like system; (4) specify design variables, practical constraints, and optimization criteria; (5) build a literature-anchored demonstration over the 80–150 °C domain; (6) test a fast surrogate against the transparent reference model; (7) propagate input uncertainty into net-power predictions; and (8) define an open implementation architecture suitable for DWSIM/Python workflows and future industrial validation.

Research Questions

RQ1: What minimum set of source, sink, working-fluid, component, and property-model inputs is required for a reproducible sub-150 °C Kalina-cycle design?

RQ2: How should thermodynamic-property verification, component verification, and cycle-level validation be sequenced before optimization results are accepted?

RQ3: How do heat-source temperature, ammonia mass fraction, high-side pressure, heat-exchanger pinch, component efficiencies, and sink temperature interact to determine feasible net power and efficiency?

RQ4: Can a machine-learning surrogate reproduce the outputs of a transparent thermodynamic reference model with sufficient accuracy for rapid screening while preserving applicability-domain controls?

RQ5: How materially does uncertainty in source and component conditions widen predicted net-power outcomes at a representative low-temperature design point?

Research Hypotheses

H1: The net performance optimum will require source-temperature-dependent ammonia concentration and high-side pressure rather than one universal operating pair.

H2: Reducing exchanger minimum approach temperature will generally increase heat recovery and net power, but the benefit will be constrained by exchanger area, fouling, and practical design margins.

H3: A surrogate trained only on verified feasible-cycle outputs can reproduce the transparent model with high predictive fidelity inside the sampled design domain.

H4: Thermodynamic-property and operating uncertainty will produce a non-negligible spread in predicted power, making interval reporting preferable to single-point performance claims.

LITERATURE REVIEW

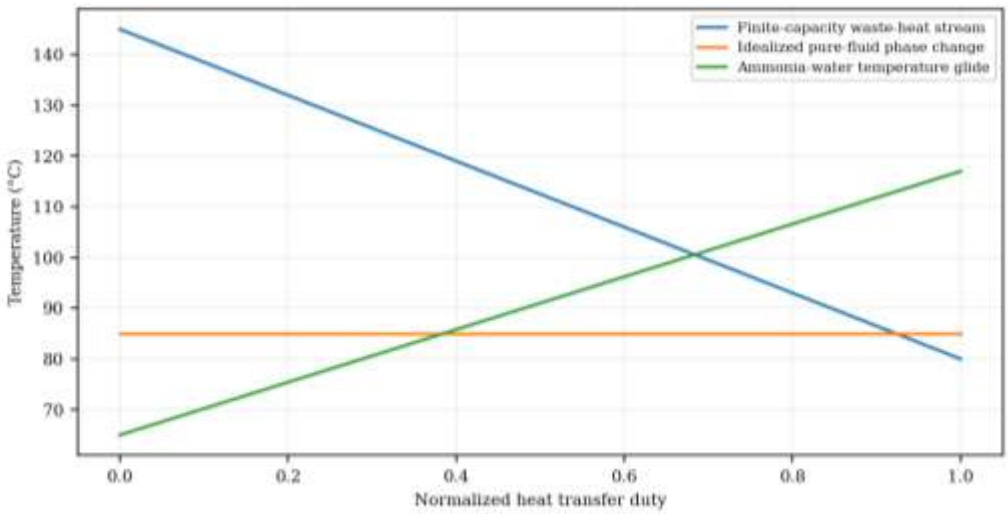
Kalina Cycle and Low-Temperature Heat Recovery

The conceptual origin of the Kalina cycle lies in the use of a multicomponent working fluid to modify boiling and condensation temperature profiles. Kalina (1984) introduced the bottoming-cycle concept for both combined-cycle systems and low-temperature heat sources. Unlike a pure working fluid, an ammonia–water mixture can boil and condense over a temperature range at a given pressure. This creates an additional design degree of freedom (Abdullah Mohammad, 2023; Debasish, 2023; Md Kaium, 2023): the mixture can be selected so that the working-fluid temperature profile follows the declining temperature of a finite-capacity source more closely (Mst Kaniz, 2022; Nishat & Mst Kaniz, 2022; Shaiful et al., 2022).

The benefit is best interpreted through exergy rather than through a blanket statement that Kalina is always superior to an organic Rankine cycle. Zhang et al. (2012) reviewed energy/exergy analyses, cycle configurations, property correlations, and practical concerns and showed that published comparisons depend on the selected source/sink and model assumptions. Larsen et al. (2014) and Nguyen et al. (2014) further demonstrated that split-cycle arrangements can reduce heat-recovery irreversibility by changing ammonia concentration through the heat-addition process, but at the cost of additional complexity. This literature supports a methodology that compares feasible designs under common boundary conditions instead of assigning a universal ranking.

For very low heat-source temperatures, the heat exchanger becomes as important as the turbine (Abdullah Mohammad, 2023; Debasish, 2023; Md Kaium, 2023). Golubovic et al. (2007) showed that KCS-11 performance is sensitive to ammonia fraction and pressure. Ogriseck (2009) demonstrated integration into an industrial CHP context, and Matsuda (2013) documented the practical motivation for around-120 °C industrial sources. Collectively, these studies suggest that the design problem should be expressed as source–cycle matching with explicit pinch and heat-utilization constraints.

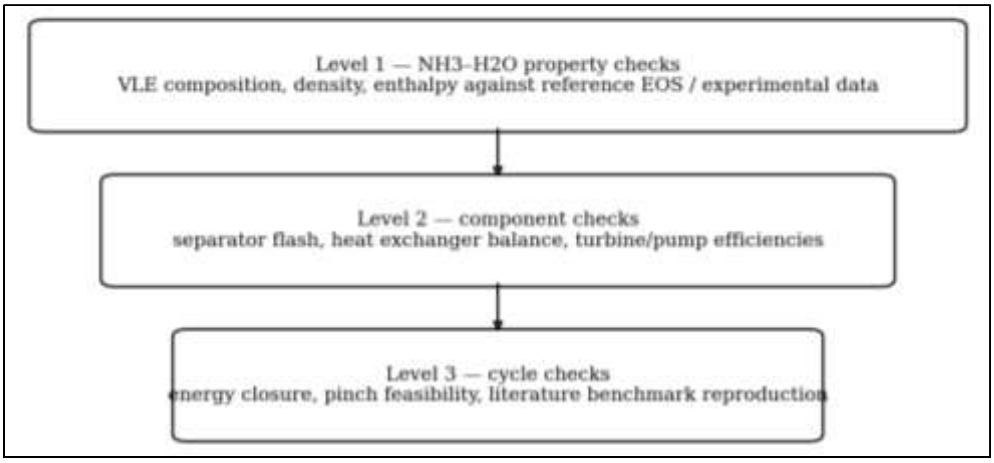
Figure 4: Conceptual Effect of Ammonia–Water Temperature Glide on Source Matching



Ammonia–Water Thermodynamic Property Requirements

Accurate ammonia–water thermodynamics are a prerequisite to credible Kalina design because the separator, evaporator, condenser/absorber, and recuperator all cross or approach two-phase regions. Tillner-Roth and Friend (1998a) compiled and assessed the available measurements and identified the data foundation needed for an equation of state. Tillner-Roth and Friend (1998b) then formulated a Helmholtz-free-energy model covering vapor and liquid phases to high pressure and reported typical reference uncertainties of approximately ±0.01 in equilibrium mole fractions, around ±0.3% in single-phase density, and ±200 J/mol in enthalpy (Md Mahamud Pervaz, 2023; Mohammad Abir Chowdhury, 2023; Mohammad Badrul & Md. Mominul, 2023). Those reference uncertainties are small enough to support engineering modeling but large enough to matter when cycle net efficiency is only several percentage points (Ashrafuzzaman, 2024; Debasish, 2024; Nishat, 2023). Property packages can also differ more than the reference uncertainty if they use different activity-coefficient models, cubic equations, or binary-interaction parameters (Md Anisur Rahman, 2024; Md Kaium, 2024; Md. Shakhawat & Md, 2024). Therefore, model validation must be performed at the actual ranges of temperature, pressure, and ammonia composition traversed by the proposed flowsheet (Nishat & Jahanara, 2024; Tonay et al., 2024; Uddin & Risha, 2024). Agreement at room-temperature single-phase points is insufficient if the cycle depends on high-pressure two-phase flash calculations. An open implementation may use DWSIM because the platform is free/open-source and supports steady-state and dynamic process simulation. However, openness of the simulator is not itself evidence that a particular ammonia–water property package is valid. The selected model and interaction parameters must still pass the property-level verification suite before the process results are accepted (Debasish, 2025a, 2025b; Jannatul, 2025).

Figure 5: Hierarchical Verification and Validation Strategy

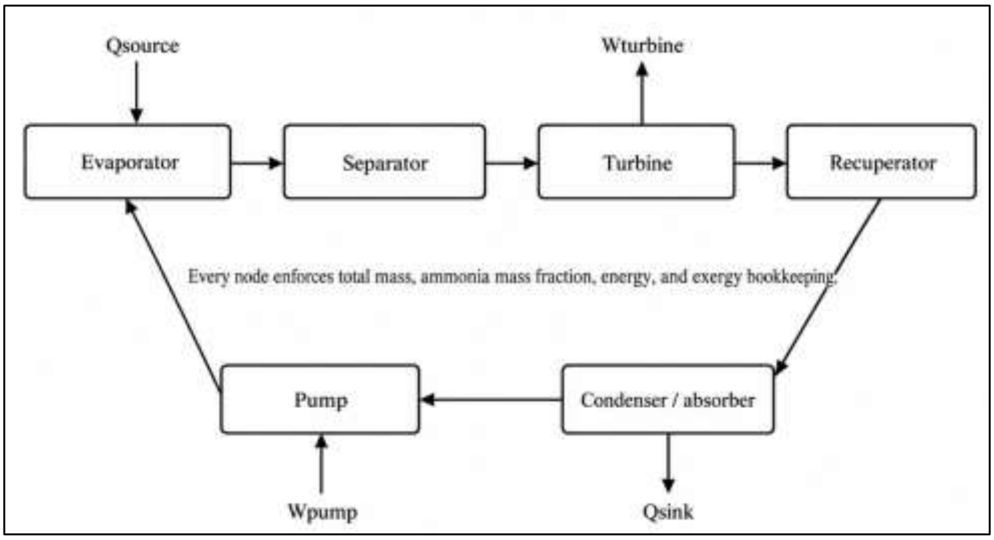


Heat Integration, Exergy, and Off-Design Operation

Kalina performance is inseparable from heat integration. Nguyen et al. (2014) showed through exergy analysis that changing ammonia concentration during heat addition can improve source matching and reduce irreversibility in the heat-recovery section. Larsen et al. (2014) similarly used multi-variable optimization for a split-cycle and reported a performance gain relative to the reference configuration under the specific marine-engine boundary conditions. Such improvements do not transfer automatically to sub-150 °C industrial sources, but the underlying lesson is general: cycle topology and exchanger network should be optimized together (Md Anisur Rahman, 2025; Md Arif Uz et al., 2025; Md Kaium, 2025).

Off-design performance matters because industrial waste heat rarely remains perfectly stationary. Li et al. (2016) studied a low-temperature geothermal Kalina system under variations in source temperature, source flow, and sink temperature and evaluated a sliding-pressure control strategy. The same logic applies to industrial recovery (Md Mahamud Pervaz, 2025; Mohammad Abir Chowdhury, 2025; Mohammad Badrul, 2025): a design optimized for a 120 °C nominal source may spend significant operating hours at 105 or 135 °C, with correspondingly different optimal pressure and working-fluid flow (Nishat, 2025; Nuzhat Sadia, 2025; Sadia, 2025). Exergy analysis provides a useful diagnostic because it identifies where finite temperature differences, non-isentropic expansion, mixing, and condensation destroy work potential. The method developed here therefore calculates both energy and exergy metrics and treats the minimum approach temperature as an explicit design constraint rather than a post-processing check (Tonay, 2025).

Figure 6: Mass, Species, Energy, and Exergy Bookkeeping Network



Machine Learning and Performance Surrogates

The nonlinear thermodynamics of ammonia–water systems make repeated optimization expensive. Chen and Yuan (2023) showed that ANN surrogates can reproduce a thermal model closely when trained with sufficient data, while a thermally constrained architecture improves generalization when data are limited. Chen et al. (2025) advanced this approach by embedding thermodynamic constraints and anomaly detection into machine-learning models for ammonia–water thermal systems. Their results reinforce a crucial methodological rule: a surrogate should be trained on verified physics-model outputs and should be rejected when it violates conservation or leaves the domain represented by the training set.

In the present workflow the surrogate is intentionally simple: a random forest predicts net power from the design variables generated by the transparent reference model. This model is not intended to establish the best machine-learning algorithm. It demonstrates how a fast screening layer can be evaluated through held-out cross-validation, feature importance, physical plausibility checks, and explicit input bounds.

THEORETICAL AND CONCEPTUAL FRAMEWORK

The conceptual framework treats Kalina-cycle design as a chain of evidence rather than as a single optimization problem. The first layer is the physical source: temperature–time history, mass flow or heat-capacity rate, composition, fouling tendency, allowable outlet temperature, pressure/backpressure constraints, and shutdown/transient behavior. The second layer is thermodynamic representation: the ammonia–water property model and component equations. The third layer is constrained design: decision variables are varied only inside a physically and operationally feasible domain. The fourth layer is prediction and optimization: response surfaces or surrogates accelerate search without bypassing the validated solver. The final layer is decision reporting: nominal performance is accompanied by uncertainty, constraint status, model version, and applicability-domain information. This structure also distinguishes verification from validation. Verification asks whether the equations were solved correctly and whether mass, ammonia species, energy, and exergy balances close numerically. Validation asks whether the selected physical models reproduce external reference behavior to an acceptable tolerance. A cycle solver can be numerically perfect and still invalid if its ammonia–water VLE model is inaccurate in the region of interest.

METHOD

The study uses a computational methodology-development design. It has two distinct evidence layers. The first is source-derived: peer-reviewed Kalina-cycle studies, NIST ammonia–water reference-property work, and open-simulator documentation define the scientific and implementation requirements. The second is a synthetic numerical demonstration constructed solely to show how the methodology behaves. The synthetic layer is not described as industrial plant data, and its fitted response surfaces are not proposed as new universal Kalina correlations.

The reference implementation covers a heat-source inlet range of 80–150 °C and a water-cooled sink of 20–35 °C. The cycle is represented by a KCS-11-like single-pressure architecture with pump, recuperation, heat addition, phase separation, expansion, mixing/absorption, condensation, and internal recovery. The exact number of recuperators, separators, and splits is intentionally configurable because published Kalina variants differ materially.

Figure 7: Design Variables and Sampled Bounds in the Demonstration Study

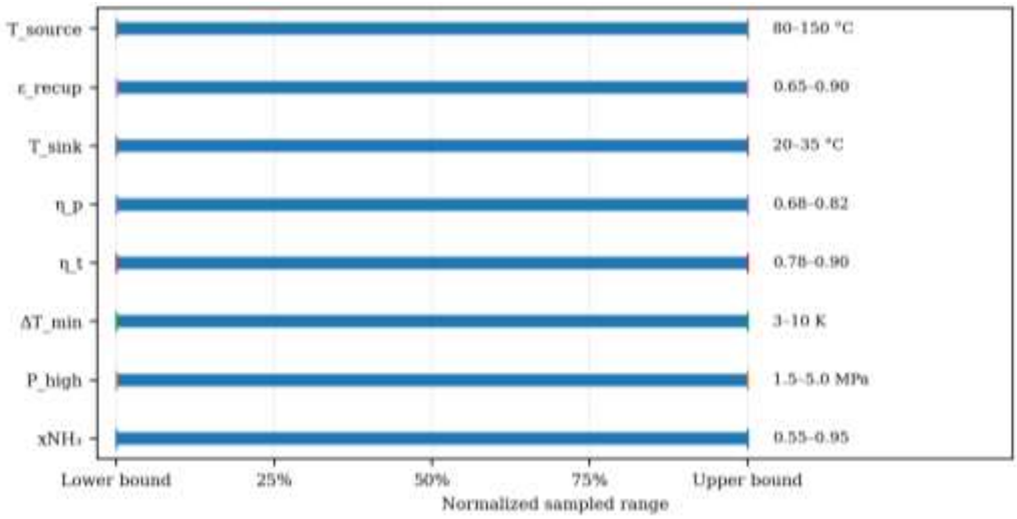


Table 1. Boundary Conditions and Design Variables

Parameter	Demonstration range	Role
Heat-source inlet temperature	80–150 °C	Measured/project-specific in real deployment
Available heat duty	2–8 MW in synthetic DOE	4 MW for representative optimized cases
Heat-sink temperature	20–35 °C	Cooling-water/ambient boundary
NH_3 mass fraction	0.55–0.95	Optimization variable
High-side pressure	1.5–5.0 MPa	Optimization variable
Minimum approach ΔTmin	3–10 K	Heat-exchanger feasibility constraint
Turbine isentropic efficiency	0.78–0.90	Uncertain component input
Pump isentropic efficiency	0.68–0.82	Uncertain component input
Recuperator effectiveness	0.65–0.90	Internal heat-recovery input

Open Thermodynamic Validation Protocol

The property-validation suite should be implemented before cycle optimization. At minimum it should contain: (i) saturation and VLE composition points spanning the operating pressure/composition domain; (ii) single-phase density and enthalpy checks; (iii) bubble/dew continuity tests; (iv) enthalpy

monotonicity and phase-consistency checks; and (v) flash convergence tests near the separator and condenser operating regions. Reference data and the Helmholtz model of Tillner-Roth and Friend (1998a, 1998b) provide the primary validation basis.
Component verification then applies conservation checks. Every component must close total mass and ammonia species balances to a specified numerical tolerance, and the full-cycle energy residual should be several orders of magnitude smaller than the recovered heat duty. Heat exchangers should additionally be discretized so that the minimum approach temperature is verified along the entire composite curve, not only at terminal temperatures.
Cycle-level validation is the third stage. Published benchmark points should be reproduced using the same source/sink temperatures, ammonia fraction, pressure, component efficiencies, pressure-drop assumptions, and architecture. A performance match obtained by changing multiple unreported assumptions is not a valid benchmark. In this article, a three-point dataset reported by Tiktas (2025), attributed there to an experimental dataset of Sun et al., is used only as an external consistency check for the reduced-order demonstration.

Table 2. Validation Hierarchy and Acceptance Logic

Level	Test	Reference	Acceptance logic
Property	VLE composition	Reference EOS / measured dataset	$\lvert\Delta x\rvert$ within predeclared tolerance
Property	Density and enthalpy	Reference values	Relative/absolute error within tolerance
Component	Mass/species balance	Conservation equations	Normalized residual < solver tolerance
Component	Heat exchanger	Segmented T–Q profile	$\Delta T \geq \Delta T_{min}$ everywhere
Cycle	First-law closure	Whole-cycle balance	Residual negligible vs. heat input
Cycle	Published benchmark	Matched boundary conditions	Error reported without retuning hidden inputs
Surrogate	Held-out test set	Validated solver outputs	R^2, MAE, RMSE + physical checks

Transparent Reduced-Order Demonstration Model
To make the article numerically reproducible without embedding a proprietary property library, the demonstration uses a transparent reduced-order model. Its net efficiency is constructed from the Carnot fraction multiplied by a smooth second-law utilization factor that varies with source temperature, ammonia concentration, high-side pressure, pinch, component efficiencies, and recuperation. The optimum ammonia concentration and pressure are allowed to shift with source temperature. Heat-recovery fraction is separately represented so that a design can have high internal cycle efficiency but poor source utilization, or vice versa.
The reduced-order formulation is intentionally modest. It produces low-temperature efficiencies in the same order as published KCS values but is not calibrated as an ammonia–water EOS. Any engineering use must replace this layer with validated VLE/enthalpy calculations. The model's value here is methodological: every assumption is visible, parameter ranges can be stress-tested, and surrogate/uncertainty workflows can be demonstrated without mislabeling synthetic outputs as measured performance.
Design of Experiments and Optimization
A 2,400-case random design is generated across the ranges in Table 1. Each point produces net efficiency, heat-source utilization, recovered heat, net power, exergy efficiency, source outlet temperature, a temperature-glide matching score, and a feasibility flag. Representative optimized designs at fixed source temperatures are then obtained by a transparent grid search over ammonia mass fraction, high-side pressure, and minimum approach temperature while holding the other component assumptions at stated values.

The optimization objective in the demonstration is net electrical power from a 4 MW available heat source. This choice prevents the optimizer from maximizing efficiency by recovering an impractically small fraction of the available heat. A production study could use multi-objective optimization over net power, exergy efficiency, heat-exchanger area/cost, ammonia inventory, and economic metrics.

Surrogate Modeling and Applicability Domain

A random-forest regressor is trained on 75% of the synthetic design set and evaluated on a 25% held-out subset. Inputs are source temperature, ammonia fraction, high-side pressure, pinch, turbine/pump efficiency, sink temperature, recuperator effectiveness, and available heat duty. The surrogate is used only inside the sampled ranges. Predictions outside these bounds should be rejected or routed back to the thermodynamic solver.

Cross-validation statistics quantify fidelity to the transparent model rather than agreement with physical experiments. This distinction is essential: a surrogate can achieve R^2 near unity while faithfully approximating a physically incorrect parent model. Therefore, surrogate validation is the final layer, not the first layer, of the methodology.

Uncertainty Quantification

A Monte Carlo demonstration is performed for a nominal 120 °C source by perturbing source temperature, ammonia concentration, high-side pressure, pinch, turbine/pump efficiency, sink temperature, and recuperator effectiveness. The uncertainty distributions are illustrative. In a real project, measurement uncertainty, property-model uncertainty, heat-exchanger fouling, pressure drop, rotating-equipment maps, control uncertainty, and time variability should be estimated from project-specific evidence. The output distribution is summarized by the 5th, 50th, and 95th percentiles of net power. This interval-based reporting is particularly important at low source temperature because small changes in sink temperature or pinch can consume a large fraction of the available exergy.

DATA ANALYSIS AND PRESENTATION

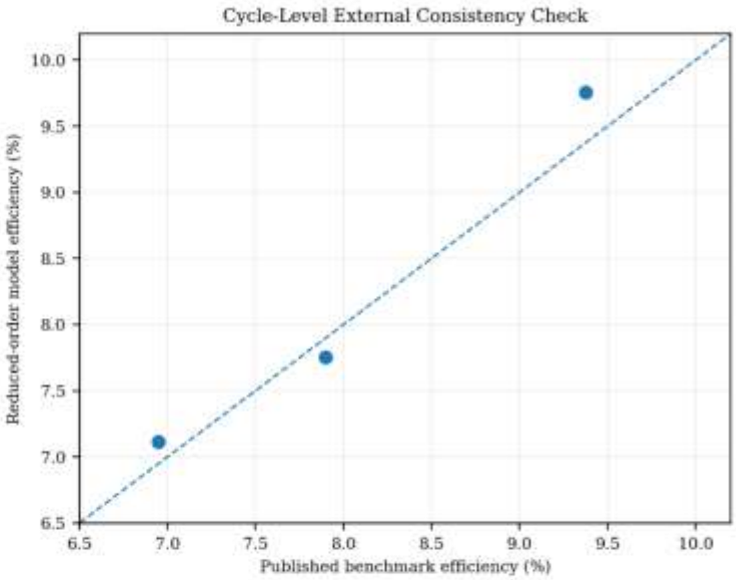
Cycle-Level Literature Consistency Check

Table 3. External Consistency Check Against Low-Temperature Benchmark Points

Source T (°C)	xNH_3	P_high (MPa)	Published η (%)	Model η (%)	Relative error (%)
99.85	0.70	2.50	6.950	7.113	2.34
112.35	0.90	3.13	7.896	7.755	1.78
149.85	0.85	4.38	9.377	9.758	4.06

The reduced-order model follows the three benchmark efficiencies with a mean relative discrepancy of 2.73% and a maximum discrepancy of 4.06%. Because the coefficients were selected to produce literature-consistent low-temperature behavior, this should be interpreted as an external consistency check rather than an independent experimental validation. The purpose of the check is to demonstrate that the synthetic study does not operate at implausible efficiency levels. The methodological implication is more important than the absolute error: the same benchmark table should be regenerated automatically whenever the ammonia–water property library, component models, or solver version changes. A regression-test failure should block subsequent optimization until the discrepancy is understood.

Figure 8: Published Benchmark Versus Transparent Reduced-Order Efficiency



Source-Temperature and Mixture Sensitivity

The response curves demonstrate that performance increases with source temperature but remains strongly conditioned by mixture composition. A concentration that is close to optimum at one source temperature is not necessarily close to optimum at another. This qualitative behavior is consistent with the KCS-11 literature and with the 100–150 °C concentration study of Intakham et al. (2025).

The model also illustrates the difference between thermal efficiency and useful project output. Net power depends on both the efficiency of the recovered heat and the fraction of source heat that can actually be transferred without violating the pinch or source-outlet constraints. Therefore, screening only by η_net can mis-rank designs that have different source utilization.

Figure 9: Synthetic Efficiency Sensitivity to Heat-Source Temperature and NH_3 Mass Fraction

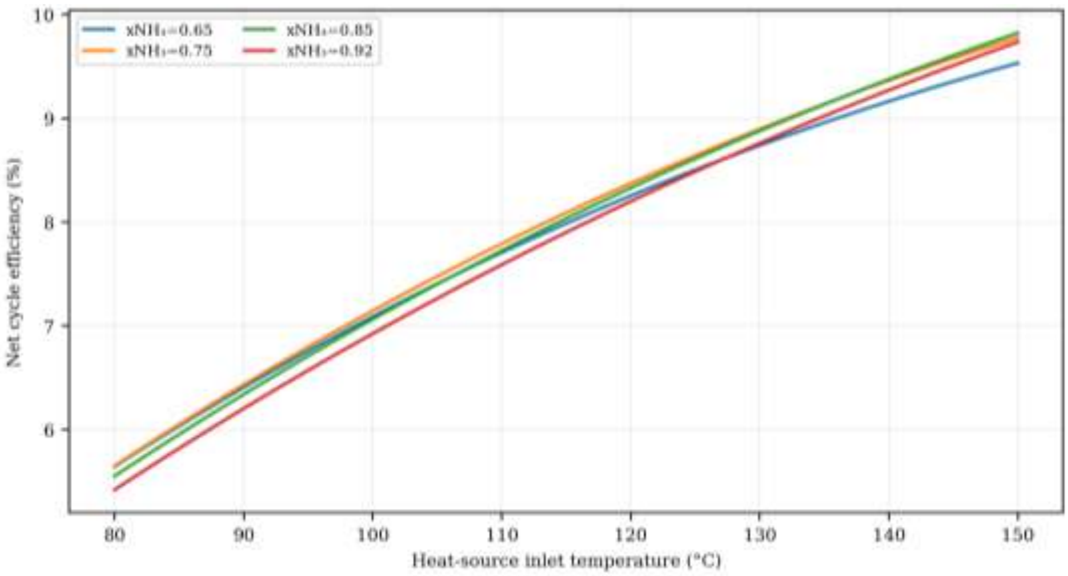
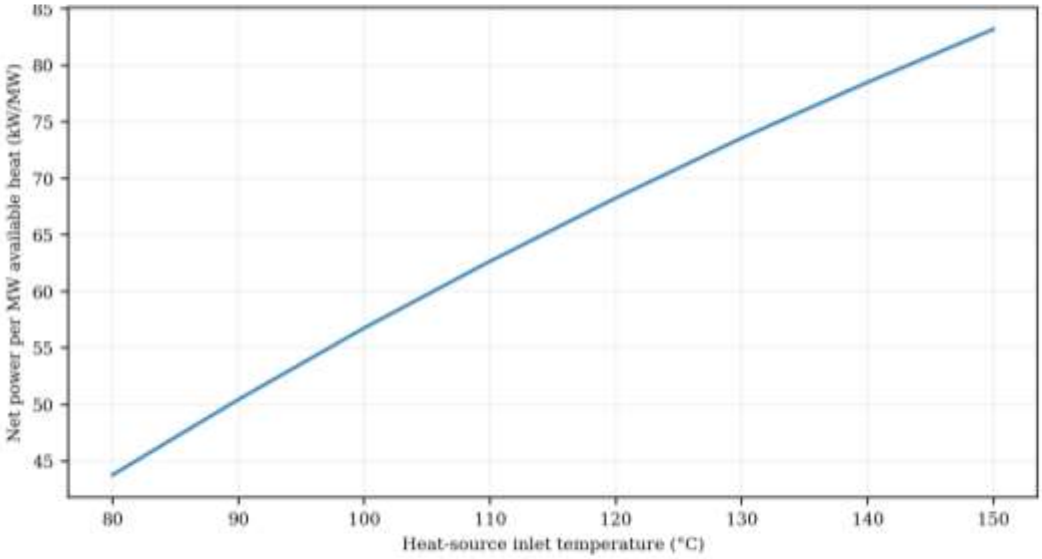


Figure 10: Optimized Specific Net-Power Potential Across 80–150 °C



Representative Optimized Designs

The optimized trajectory moves toward richer ammonia mixtures and higher pressure as source temperature rises. This is not asserted as a universal design rule; it is a transparent consequence of the demonstration equations. In a full EOS-based model, the exact trajectory will depend on phase equilibrium, turbine-inlet state, separator split, condenser pressure, pressure drops, and heat-exchanger network.

Table 4. Representative Synthetic Optimized Designs for a 4 MW Available Heat Source

Tsrc °C	xNH_3	P MPa	Pinch K	ηnet %	Wnet kW	ηex %	Heat used %	Tout °C
80	0.71	1.67	3	5.75	175	68.1	76.0	42.0
90	0.72	2.00	3	6.55	202	66.6	77.0	43.8
100	0.74	2.27	3	7.27	227	65.1	78.1	45.3
110	0.76	2.53	3	7.93	251	63.5	79.0	46.8
120	0.77	2.80	3	8.53	273	62.1	80.0	48.0
130	0.79	3.07	3	9.07	294	60.6	81.1	48.9
140	0.81	3.40	3	9.57	314	59.2	82.0	49.8
150	0.82	3.67	3	10.02	333	57.8	83.1	50.3

The key methodological result is that the optimization output can be plotted as a trajectory rather than reported as one isolated “optimal” point. This makes it possible to design control logic or an off-design schedule that responds to seasonal or process-driven changes in source temperature.

Figure 11: Source-Temperature Dependence of Synthetic Optimal NH_3 Fraction and High-Side Pressure

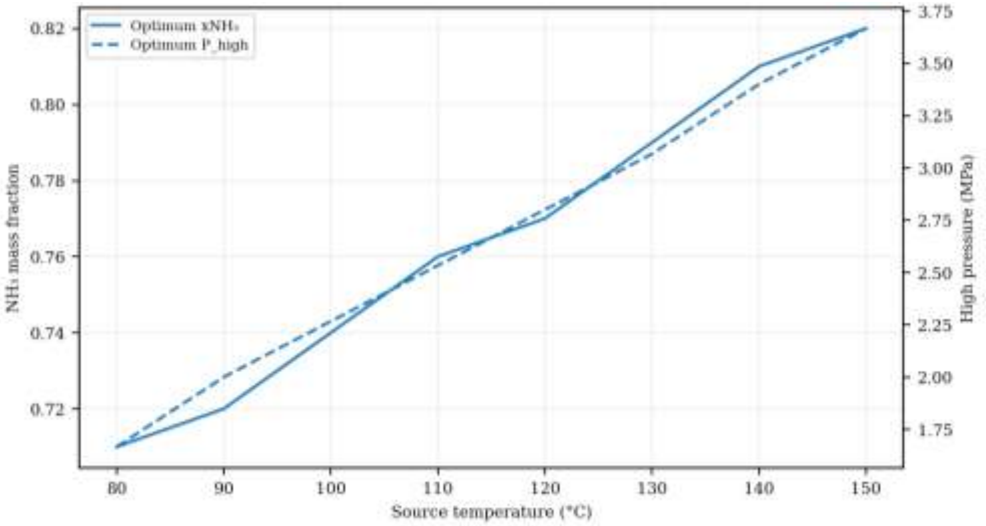
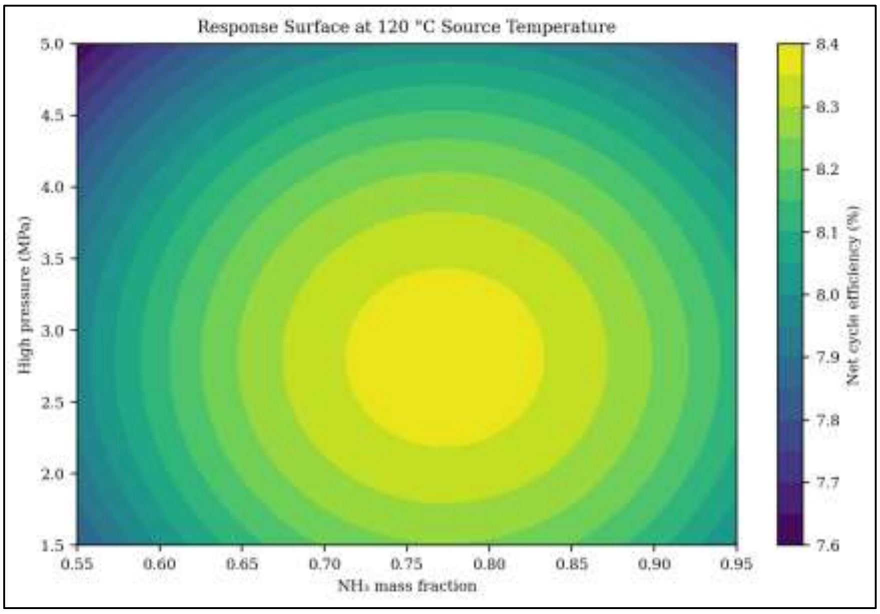


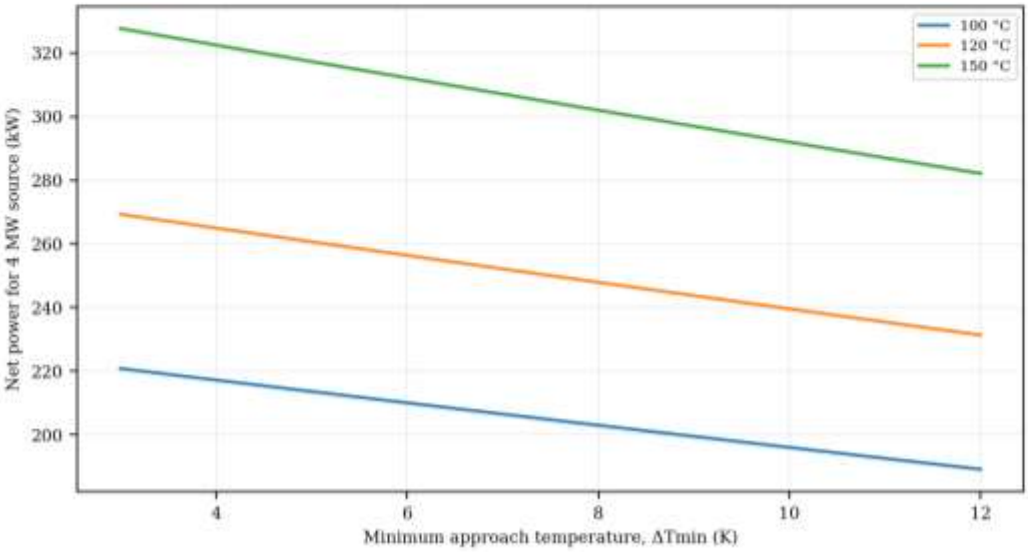
Figure 12: NH_3 Fraction–Pressure Response Surface at a 120 °C Source



Heat-Exchanger Constraint Sensitivity

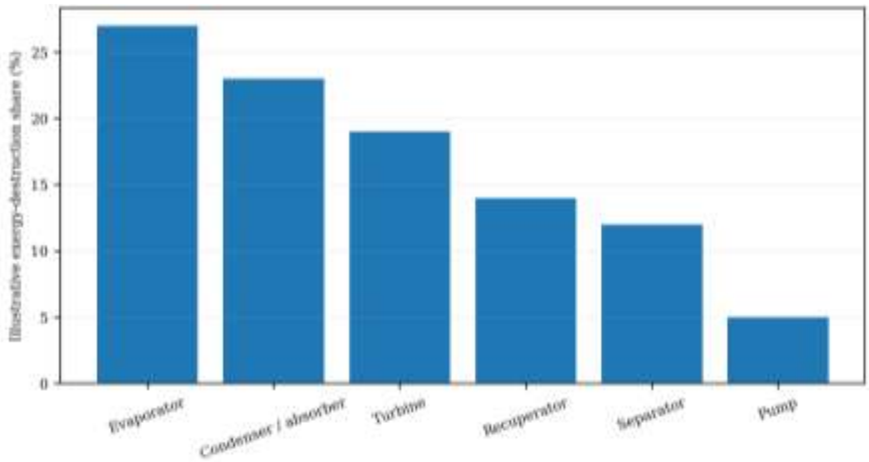
The pinch-sensitivity curves show a systematic reduction in recoverable net power as ΔTmin increases. The effect is more consequential at the lower source temperatures because the available temperature span is already small. This is why an attractive thermodynamic design can become uneconomic when exchanger area, fouling allowance, or approach-temperature constraints are introduced. A practical design should therefore report the selected pinch together with the assumed overall heat-transfer coefficient, fouling resistance, allowable pressure drop, and exchanger-area estimate. The methodology intentionally treats ΔTmin as a design input rather than hiding it inside the solver.

Figure 13: Synthetic Net-Power Sensitivity to Minimum Heat-Exchanger Approach Temperature Exergy Diagnosis



An exergy budget is included to demonstrate how the workflow identifies where additional model detail or capital investment may be most valuable. The particular shares shown in Figure 14 are not measurements. In a validated flowsheet, exergy destruction would be calculated directly from stream enthalpy/entropy states and compared across the evaporator, condenser/absorber, turbine, recuperators, separator/mixer, and pump.

Figure 14: Base-Case Exergy-Destruction Allocation



Published Kalina studies have repeatedly shown that the heat-recovery train, condenser, and expansion process can contain important irreversibilities, but the dominant component is configuration-dependent (Nguyen et al., 2014). This reinforces the need to calculate exergy locally rather than import a component ranking from another study.

Surrogate Performance

Table 5. Random-Forest Surrogate Fidelity to the Transparent Reference Model

Metric	Value	Unit
Held-out cases	600	—
R^2	0.9825	Dimensionless
MAE	11.65	kW
RMSE	15.33	kW

The held-out surrogate results show high fidelity to the transparent parent model, with R^2 = 0.9825, MAE = 11.6 kW, and RMSE = 15.3 kW. These metrics establish computational approximation quality only. They do not validate the thermodynamics of the parent model. Feature importance is dominated by available heat duty and source temperature, followed by variables that influence the second-law utilization and heat-recovery fraction. Such importance rankings should not be interpreted causally because tree-based importance can depend on feature ranges and correlations. Their value is diagnostic: unexpected dominance by a weak or arbitrary input can reveal errors in the training data or model formulation.

Figure 15: Held-Out Surrogate Prediction Versus Transparent-Model Net Power

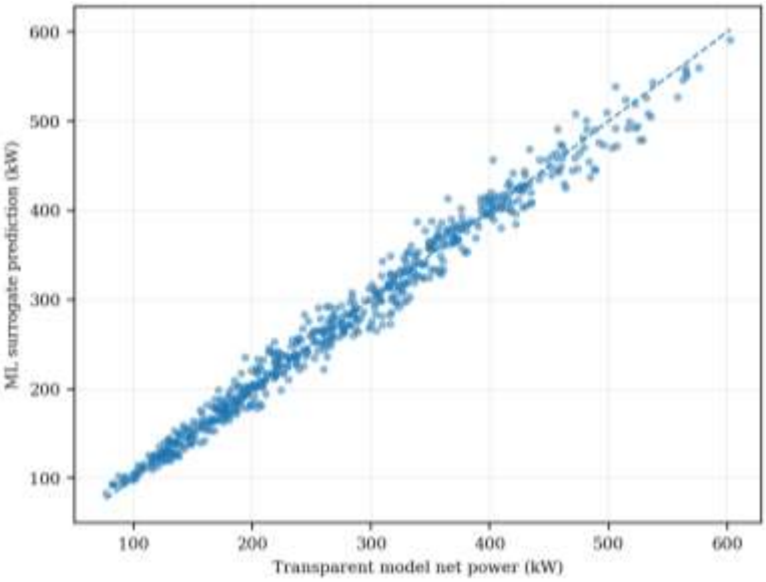
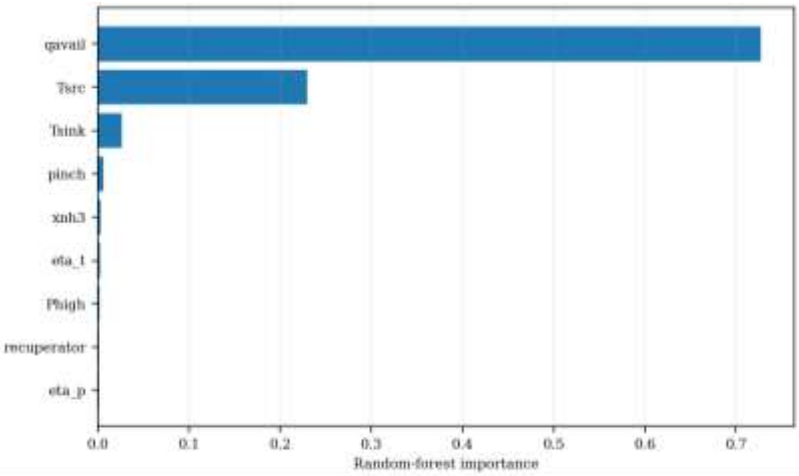


Figure 16: Random-Forest Feature Importance for Net-Power Screening



Uncertainty Results

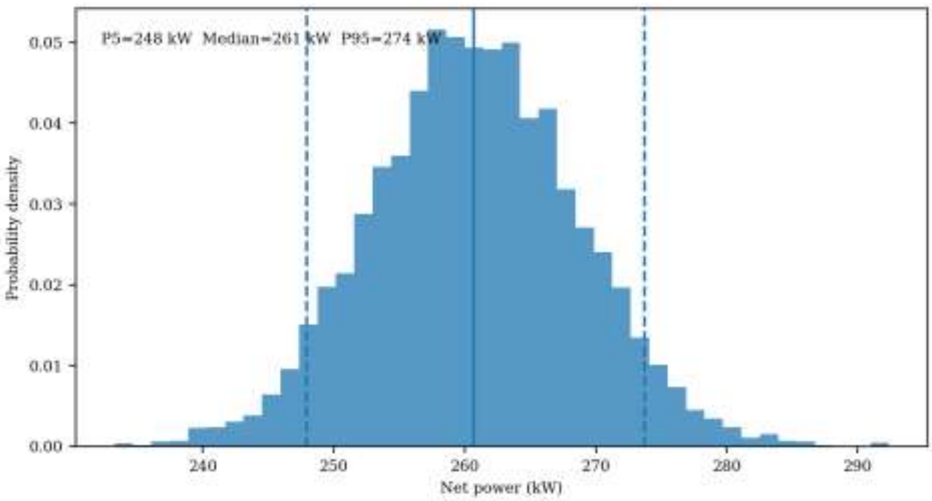
Table 6. Monte Carlo Net-Power Distribution at the 120 °C Base Case

Statistic	Net power	Unit
P5	247.9	kW
Median	260.7	kW
P95	273.7	kW
P95–P5 width	25.8	kW
Relative interval width	9.9	% of median

The Monte Carlo distribution spans approximately 248 to 274 kW between the 5th and 95th percentiles, with a median near 261 kW. The width is generated by modest uncertainty in source temperature, working-fluid composition, pressure, pinch, component efficiencies, sink temperature, and recuperation. This result shows why nominal values alone can give a false impression of precision in low-grade heat recovery.

In project use, uncertainty should be decomposed by source. Thermodynamic-property model uncertainty should be treated separately from sensor uncertainty, source variability, equipment-map uncertainty, fouling, and control variability. That separation allows the engineer to determine whether additional plant measurement, a better property model, or more conservative equipment sizing would reduce decision uncertainty most effectively.

Figure 17: Monte Carlo Net-Power Distribution for the 120 °C Base Case.



DISCUSSION

"Open" in this study means that the governing equations, input ranges, property-model identity, solver settings, validation cases, optimization logic, random seeds, and post-processing are inspectable and reproducible. It does not mean that every open-source property model is automatically suitable. DWSIM provides a useful open flowsheet environment, but a project must still verify the selected ammonia–water thermodynamics against accepted reference data. "Validated" is likewise hierarchical. A credible claim requires evidence at the property level, component level, and cycle level. A machine-learning surrogate cannot raise the validation level above that of its training solver. Conversely, an accurate property package does not guarantee a correct cycle if heat-exchanger pinches, separator phase equilibrium, pressure drops, or mixer balances are implemented incorrectly. The methodology therefore treats validation as a chain in which the weakest unverified layer limits the credibility of the final performance prediction. The three-point literature consistency check in this paper is deliberately described narrowly. It verifies that the transparent demonstration model occupies the expected efficiency scale; it does not transform the reduced-order equations into a validated design tool. The full proposed workflow reaches engineering validation only after the reference implementation is replaced with a qualified ammonia–water thermodynamic solver and benchmarked against sufficiently detailed experimental or plant data.

Design Implications for Sub-150 °C Industrial Heat

The results reinforce four practical implications. First, the heat sink is almost as important as the heat source at low temperature because condenser approach and ambient/cooling-water conditions determine the available temperature lift. Second, ammonia concentration should be optimized jointly with pressure and topology rather than selected from a rule of thumb. Third, heat-exchanger feasibility can dominate the result; low ΔTmin improves thermodynamics but usually increases area, cost, and fouling sensitivity. Fourth, off-design schedules should be designed alongside the nominal cycle because industrial sources vary over time.

The methodology also discourages direct comparison of isolated efficiencies from different papers.

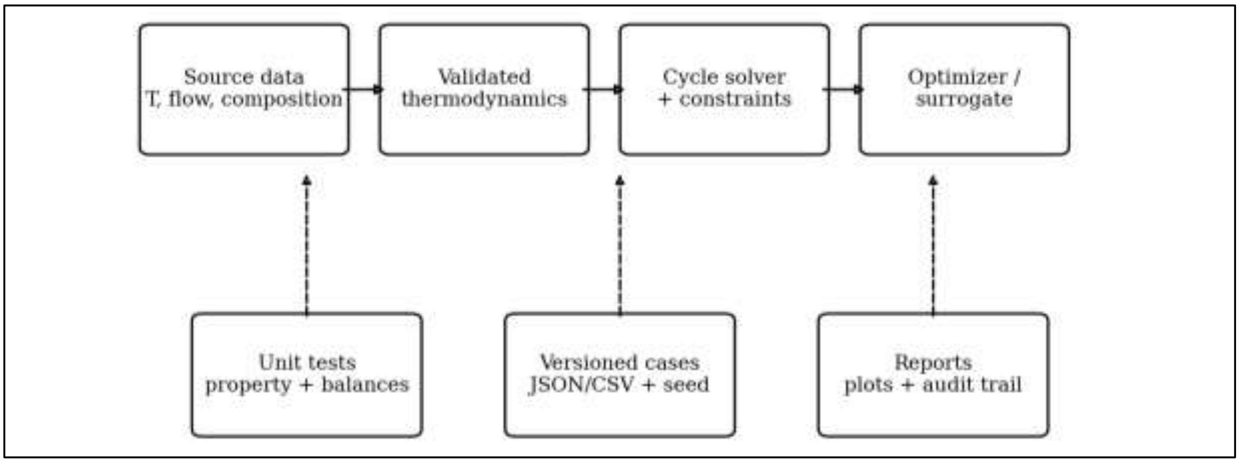
Ogriseck (2009), Golubovic et al. (2007), Larsen et al. (2014), and other studies examine different source temperatures, sink conditions, architectures, pressure drops, and component efficiencies. A fair comparison requires a common boundary-condition table and a common property model or, at minimum, a quantified sensitivity to property-model choice.

Open-Source and Reproducible Implementation

A practical open reference implementation can separate responsibilities. DWSIM can host the process flowsheet, unit-operation connectivity, and selected thermodynamic package. Python can manage test cases, call the solver through automation interfaces where available, perform optimization, fit surrogates, run uncertainty analysis, and generate the final report. The repository should store a machine-readable case definition for every benchmark and design point.

Each software release should rerun the validation suite automatically. Property regression tests should compare selected T–P–x states with reference values. Flowsheet tests should verify balance closure and pinch constraints. Cycle benchmark tests should reproduce published reference cases. Surrogate tests should check held-out prediction metrics and reject inputs outside the domain. Such continuous validation makes the method easier to audit than a spreadsheet or closed GUI workflow in which intermediate states are not versioned.

Figure 18: Proposed Open Implementation and Assurance Architecture



Ammonia introduces hazards that must be addressed independently of thermodynamic performance. The process design should minimize inventory, provide compatible materials, leak detection, ventilation, relief and containment strategy, and emergency response provisions appropriate to the applicable jurisdiction and facility. The literature review by Zhang et al. (2012) identifies safety and corrosion among the practical concerns associated with ammonia–water systems. These issues can materially change the preferred pressure, concentration, and equipment arrangement.

Low-temperature industrial sources can also be dirty or corrosive. Flue gas may require an intermediate loop to avoid acid condensation or deposition in the process heat exchanger; refinery or chemical streams may impose contamination or process-safety constraints; and aqueous waste streams may scale. The thermodynamic optimum should therefore be filtered through a materials and operability review before economic ranking. For fluctuating sources, controls should prevent separator instability, turbine wetness outside allowable limits, condenser/absorber maldistribution, and off-design pressure excursions. Matsuda (2013) specifically noted fluctuation as a practical issue in a low-heat power-generation application. A dynamic or quasi-steady operational model is consequently a recommended extension after the steady-state design is validated

RECOMMENDATIONS

1. Adopt the validation hierarchy as a release gate: no optimization result should be considered final until the property, component, and cycle-level test suites pass.
2. Use a reference-quality ammonia–water property formulation or a property package independently shown to reproduce the reference domain of Tillner-Roth and Friend (1998a, 1998b) over the project's

actual T–P–x envelope.
3. Optimize net power and heat-source utilization together with ammonia concentration, pressure, and heat-exchanger pinch. Do not optimize thermal efficiency alone.
4. Create off-design maps for source temperature, source flow, and heat-sink temperature. For variable plants, derive a pressure/flow/composition control schedule rather than operating at one nominal optimum.
5. Use data-driven surrogates only after parent-model validation. Enforce input bounds and conservation/thermodynamic checks, following the physics-consistent direction demonstrated by Chen and Yuan (2023) and Chen et al. (2025).
6. Report uncertainty intervals for predicted power and efficiency, and maintain a separate uncertainty budget for measurements, thermodynamic properties, component maps, pressure drop, heat transfer, fouling, and source variability.
7. Maintain an open, version-controlled repository of case definitions, model parameters, validation data, solver versions, optimization settings, random seeds, and generated reports. This makes design evolution traceable and supports independent replication.
8. Before industrial deployment, complete equipment/material compatibility, ammonia safety, HAZOP/process-safety, economic, maintainability, and environmental integration studies. A thermodynamic optimum is only one part of a deployable design.

LIMITATIONS

The principal limitation is that the numerical study is a transparent reduced-order demonstration rather than a full ammonia–water EOS-based process simulation. It intentionally does not calculate detailed phase splits, dew/bubble states, solution enthalpies, exchanger area, or pressure-drop networks from first principles. Numerical efficiency and power values should therefore not be used for equipment procurement or project finance.

The external consistency check contains only three low-temperature points reported in a later paper and attributed there to an earlier experimental dataset. It is adequate for an order-of-magnitude check, not for comprehensive validation across composition, pressure, and source temperature. A future reference implementation should use the original experimental source where available and include more operating points with complete boundary conditions.

The design-of-experiments dataset is synthetic and generated from the same transparent model used for optimization. Accordingly, the strong random-forest cross-validation statistics show surrogate fidelity only. They are not evidence that the surrogate predicts a physical Kalina plant.

Economic modeling is not included. Heat-exchanger area, metallurgy, pressure class, separator volume, turbine size, ammonia inventory, controls, installation tie-ins, downtime, and safety systems can reverse a purely thermodynamic ranking. Likewise, source fouling and temporal variability are represented only conceptually.

The framework focuses on steady-state power recovery. Combined heat-and-power, heat-pump integration, refrigeration co-production, dynamic startup/shutdown, and multi-pressure/split-cycle architectures can yield different optima. These extensions should retain the same validation and reproducibility architecture.

CONCLUSION

This study has developed an open, validation-centered methodology for the design and performance prediction of ammonia–water Kalina-cycle systems recovering industrial waste heat below 150 °C. The framework begins with source characterization, treats ammonia–water property verification as a prerequisite, enforces total mass, ammonia species, energy, exergy, and pinch constraints, and then applies optimization, surrogate modeling, and uncertainty propagation. This ordering is intentional: performance prediction is credible only to the extent that the thermodynamic and component layers underneath it have been verified and validated. The literature-anchored demonstration shows the expected qualitative behavior of a low-temperature Kalina system. Net performance rises with source temperature, but optimum ammonia concentration and high-side pressure shift across the 80–150 °C domain. Heat-exchanger approach temperature materially affects useful power, and even modest input uncertainty produces a visible range of net-power predictions. A fast surrogate can approximate the transparent parent model with high numerical fidelity, but its validity cannot exceed the validity of the parent thermodynamics. The main contribution is therefore a reproducible engineering process rather than a single efficiency number. An open DWSIM/Python implementation can make each design traceable through property tests, conservation tests, benchmark cases, optimization files, surrogate checks, and uncertainty reports. Future work should replace the demonstration equations with a reference-quality ammonia–water EOS implementation, validate against original experimental datasets and industrial measurements, add equipment cost and dynamic operation, and publish the complete case library as an auditable open benchmark for sub-150 °C waste-heat recovery.

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