

Thermodynamic Analysis, Semi-Empirical Modelling and CFD Simulation of a Scroll Expander for Micro-Solar Organic Rankine Cycle Applications

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Abstract

The increasing need for decentralized renewable electricity has created interest in converting low- and medium-temperature heat into useful power at small scales. The uploaded thesis investigates the suitability of an Organic Rankine Cycle (ORC) for micro-solar thermal applications and develops a scroll expander as a positive-displacement expansion device for approximately 10 kW-scale systems. The work combines thermodynamic cycle analysis, working-fluid screening, semi-empirical scroll-expander modelling, dimensional analysis and computational fluid dynamics (CFD). Five candidate fluids—R134a, isobutane, R245fa, R123 and n-pentane—are examined under source-temperature conditions representative of moderate-temperature solar thermal systems. The cycle analysis compares basic and regenerative ORC configurations using first- and second-law approaches. The study identifies an optimum pressure ratio for each working-fluid and inlet condition and reports that regeneration improves cycle performance by recovering expander-exhaust heat. The evaporator is identified as the dominant source of irreversibility in both cycle configurations. R245fa and R134a emerge as important candidates for subsequent expander analysis. A semi-empirical scroll model is then used to investigate scroll geometry, leakage, mechanical losses, heat transfer and non-dimensional performance. For an R134a case, the model predicts an isentropic-efficiency range of approximately 72–76% over a pressure-ratio range of 2.5–4.5. The study further develops an Ns – Ds representation of scroll-expander geometries and identifies a distinct operating domain for scroll machines. Finally, a transient two-dimensional CFD model using dynamic meshing is used to resolve spatial variations of flow and thermal properties. The CFD results demonstrate the value of high-fidelity simulation for qualitative design assessment, leakage-model development and refinement of semi-empirical designs, while also revealing the limitations associated with two-dimensional modelling and omission of mechanical losses.

Keywords: Organic Rankine Cycle; Solar Thermal Energy; Scroll Expander; Working Fluid Selection; Semi-Empirical Modelling; CFD; Dynamic Meshing; Exergy; Specific Speed; Specific Diameter.

1. Introduction

The energy system is undergoing a gradual transition toward renewable and distributed generation. The thesis motivating this paper notes that energy demand is expected to continue increasing and that India combines high energy demand with significant solar-resource

availability. Solar thermal conversion is particularly relevant when the available heat can be concentrated and supplied to a thermodynamic power cycle. However, the conversion of solar energy into electricity is constrained by the relatively low grade and variable nature of the solar heat source. The thesis explains this limitation using the second law of thermodynamics: a thermal source at a comparatively low temperature has a lower theoretical work potential than a high-temperature fossil-fuel source.

For solar thermal power, concentrating solar power (CSP) systems convert solar radiation into heat and then use a thermodynamic cycle to produce mechanical and electrical power. The source may be supplied by parabolic troughs, power towers, linear Fresnel reflectors or parabolic dishes. For moderate-temperature operation, parabolic trough and linear Fresnel systems can provide useful heat while avoiding some of the cost and complexity associated with very high-temperature concentrating systems. The thesis considers a source-temperature range of approximately 370–420 K for the principal ORC analysis, with an ambient temperature of 303 K and a condenser saturation temperature corresponding to 308 K.

Conventional steam Rankine systems become increasingly difficult to justify as power output and source temperature decrease. The source thesis identifies poor scalability, high capital cost, water consumption, possible wet expansion, and declining thermal efficiency as important limitations. For small-scale applications, organic fluids can be selected so that the expansion process remains in the dry region, reducing the need for extensive superheating and making positive-displacement expanders attractive. The research therefore addresses a linked problem: selecting a suitable ORC working fluid and designing an expander whose geometry and operating conditions are compatible with micro-solar thermal generation.

1.1 Research Problem

At the distributed scale, the power block must be compact, efficient, tolerant of variable operating conditions and economically practical. Turbine expanders can require high rotational speeds and become difficult to manufacture economically at very small power ratings. The thesis consequently examines positive-displacement expanders and focuses on the scroll configuration, whose orbiting motion creates a sequence of expanding working-fluid chambers.

1.2 Research Objectives

- To evaluate the suitability of ORC technology for micro-solar thermal power generation under moderate-temperature heat-source conditions.
- To screen candidate organic working fluids using thermodynamic, environmental, safety and economic considerations.
- To compare basic and regenerative ORC configurations using first-law and second-law analyses.
- To determine operating pressure ratios and expansion parameters relevant to scroll-expander design.

- To develop and apply a semi-empirical model for scroll-expander geometry, leakage, mechanical loss and heat-transfer effects.
- To use dimensional analysis and Ns – Ds representations to characterize the operating domain of scroll expanders.
- To develop a transient CFD model with dynamic meshing and compare its qualitative predictions with the semi-empirical approach.
- To identify design limitations and future research directions for optimized scroll expanders in micro-solar ORC systems.

1.3 Scope of the Study

The study is computational and thermodynamic in scope. The main cycle calculations consider R134a, isobutane, R245fa, R123 and n-pentane. The detailed scroll-expander modelling is demonstrated primarily with R134a, while the thermodynamic screening identifies R245fa and R134a as strong candidates for subsequent design work. The CFD component is two-dimensional and focuses on transient flow and thermal-field behaviour rather than a complete three-dimensional mechanical assembly.

2. Literature Review

Research on low-grade heat recovery has considered a broad range of thermodynamic cycles, including ORC, Kalina, Goswami, supercritical CO₂ and hybrid cycles. The thesis literature review emphasizes that the choice of cycle must be matched to heat-source temperature, scale and application. ORC is particularly suitable for low- and medium-temperature heat because organic fluids can be selected to provide appropriate saturation characteristics and expansion behaviour.

Working-fluid selection has been widely studied. Chen, Goswami and Stefanakos reviewed thermodynamic cycles and working fluids for low-grade heat conversion, while Tchanche et al. investigated fluid selection for low-temperature solar ORC systems. Other studies have addressed regenerative ORCs, geothermal ORCs and systematic working-fluid optimization. These studies support the thesis approach of screening fluids according to thermodynamic performance while also considering environmental impact, stability, pressure limits and safety.

Expander selection is a second critical issue. The thesis divides expanders into velocity-type machines, including axial and radial turbines, and positive-displacement machines, including scroll, screw and rotary-vane expanders. The literature data reproduced in the thesis show that small-scale scroll expanders can achieve useful isentropic efficiencies while operating at substantially lower rotational speeds than micro-turbines. Experimental work by Wang et al. on R134a, for example, reported approximately 66–75% efficiency over a pressure-ratio range of 2.5–5.0.

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2.1 Selected Literature Evidence

Study	Expander / Fluid	Reported performance in thesis	Relevance
Yamamoto et al.	Radial turbine / R123	48% isentropic efficiency; 0.15 kW	Illustrates small turbine scale
Kang	Radial turbine / R245fa	78.7%; 32.7 kW; 63,000 rpm	High-speed turbine reference
Zanelli & Favrat	Scroll / R134a	63–65%; 1.0–3.5 kW; 2400–3600 rpm	Scroll-expander evidence
Mathias et al.	Scroll / R123	67–83%; 1.2–1.75 kW; 3670 rpm	Scroll performance range
Wang et al.	Scroll / R134a	70–77%; 0.5–0.8 kW; 1015–3670 rpm	Experimental comparison
Jradi et al.	Scroll-related micro solar/biomass ORC	75% expander efficiency; pressure ratio 4.6	Micro-ORC relevance

Table 1. Selected expander-performance evidence reproduced/summarized from the uploaded thesis literature review.

2.2 Research Gap

The literature demonstrates that ORC technology and scroll expanders have been investigated separately and in experimental combinations, but the thesis identifies a need for a systematic design methodology linking cycle thermodynamics, working-fluid behaviour, scroll geometry and detailed flow physics. A key limitation of semi-empirical modelling is that it predicts outlet states and overall performance without resolving the spatial distribution of pressure, temperature, velocity and density inside the moving chambers. Conversely, CFD provides richer spatial information but is substantially more computationally demanding and is difficult to implement for a continuously changing scroll domain. The present work addresses this gap by using the two methods in sequence: semi-empirical modelling for rapid design-space exploration and CFD for detailed flow-field interpretation.

3. Materials and Methods

3.1 ORC Thermodynamic Model

The thermodynamic analysis considers two cycle configurations: a basic ORC and a regenerative ORC. In the basic configuration, the working fluid is pumped from condenser pressure to evaporator pressure, heated by the solar-derived heat-transfer fluid, expanded in the expander, and condensed before returning to the pump. In the regenerative configuration, a regenerator transfers part of the expander-exhaust heat to the pressurized working fluid before it enters the evaporator.

The principal assumptions used in the thesis cycle analysis are steady operation, a 5°C subcooling condition at the pump inlet, 5% pressure drop in the evaporator, condenser and

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regenerator, and pump and expander isentropic efficiencies of 0.8. The ambient temperature is 303 K. The condenser saturation temperature is set at 308 K, i.e., 5°C above ambient. The heat-source temperature is varied from 370 K to 420 K in 10 K increments, and the pressure ratio is varied up to 16.

3.2 Working Fluids

Fluid	Type in thesis	Normal boiling point (°C)	Critical temperature (°C)	Critical pressure (MPa)	Latent heat (kJ/kg)	ASHRAE class
R134a	Isentropic	-26.3	101.5	4.06	155.4	A1
Isobutane	Dry	-11.7	134.7	3.64	303.4	A3
R245fa	Isentropic	15.3	157.5	3.64	177.1	B1
R123	Isentropic	27.8	183.7	3.66	168.4	B1
n-Pentane	Dry	36.0	196.5	3.36	349.0	A3

Table 2. Thermophysical and safety properties of the principal candidate working fluids reported in the thesis.

The fluid-selection procedure considers the shape of the saturated-vapour curve, operating pressure, enthalpy drop, chemical stability, environmental characteristics, safety and cost. The thesis classifies water as a wet fluid because of its negative saturated-vapour-line slope, while R134a, R245fa and R123 are treated as approximately isentropic fluids and n-pentane and related fluids as dry fluids. This distinction is important because wet expansion can introduce liquid droplets and potentially damage or reduce the performance of an expander.

3.3 First- and Second-Law Performance Measures

The principal first-law performance indicator is cycle thermal efficiency:

$$\eta_{th} = W_{net} / Q_{in}$$

where W_{net} is the net cycle work and Q_{in} is the heat supplied to the working fluid.

For expander assessment, the isentropic efficiency compares the actual enthalpy drop with the ideal isentropic enthalpy drop. Second-law analysis is used to locate irreversibilities within the cycle. The thesis finds that the evaporator is the dominant contributor to irreversibility in both basic and regenerative configurations, while regeneration reduces evaporator irreversibility.

3.4 Semi-Empirical Scroll-Expander Model

The scroll model begins with an involute-based geometric representation. Two mating spiral wraps form enclosed chambers whose volumes vary with orbiting angle. The geometric model provides chamber volume, volume derivative and perimeter information to the thermodynamic,

leakage, heat-transfer and mechanical-loss submodels. The thesis uses a scroll-wrap thickness of 4 mm and considers operating speeds of approximately 2000–3000 rpm to avoid a gearbox. The thermodynamic submodel applies conservation of mass and energy to each chamber. Leakage is treated as a major performance loss and is evaluated through clearance-dependent flow relations. The mechanical model accounts for frictional moments at the crank pin, journal bearing, thrust bearing and Oldham coupling. Under- and over-expansion losses are evaluated by comparing the predicted exhaust state with the condenser pressure.

The overall modelling philosophy is iterative. For a specified inlet state, operating pressures, mass flow and geometric parameters are determined and the expander performance is subsequently recalculated after the estimated losses are incorporated. This makes the method computationally inexpensive enough for rapid design iteration.

3.5 Dimensional Analysis and N_s – D_s Representation

The thesis applies Buckingham's Π -theorem to express turbomachinery performance using non-dimensional groups. Specific speed (N_s) and specific diameter (D_s) are then used to represent scroll-expander operating points in a universal turbomachinery space. For the R134a design study, net power is fixed at 10 kW, scroll outlet pressure at 12.01 bar, and inlet temperature is varied from 89°C to 150°C. Aspect ratio is varied to generate alternative geometries for the same general operating requirement.

3.6 CFD Methodology

Because the scroll geometry changes continuously as the orbiting wrap moves, a conventional fixed-domain turbomachinery CFD approach is inadequate. The thesis therefore uses a dynamic-meshing strategy in ANSYS FLUENT 15.0. The scroll curves are first generated in MATLAB and then transferred to the ANSYS geometry environment. A two-dimensional model uses a 0.2 mm flank leakage gap and no radial leakage gap because of the two-dimensional formulation.

The CFD formulation solves the conservation equations for mass and energy together with momentum equations and turbulence treatment. A transient solution is required because the chamber geometry changes with orbiting position. The model is used primarily to resolve pressure, temperature, velocity and related flow-field behaviour and to compare qualitative trends with the semi-empirical model.

4. Results and Discussion

4.1 Working-Fluid Screening

The thermodynamic screening shows that water is not suitable for the investigated moderate-temperature micro-solar application because of its wet-expansion tendency. In contrast, the organic candidates exhibit dry or near-isentropic expansion behaviour. The thesis identifies R245fa and R134a as strong competitors when the fluid behaviour is considered together with the pressure ratio, specific-volume ratio, pressure difference and enthalpy drop relevant to scroll design.

The comparison of expansion properties is particularly important for scroll machines. Volume ratio influences the required chamber expansion, pressure difference influences leakage and structural loading, and the product $p \cdot v$ provides information related to flow work and the progression of expansion. The thesis observes that organic-fluid $p \cdot v$ behaviour is not necessarily monotonic throughout the complete pressure range; therefore, the scroll geometry should avoid abrupt changes in the expansion regime associated with a sign change in the $p \cdot v$ slope.

4.2 Effect of Regeneration

Regeneration increases cycle thermal efficiency because the expander exhaust can preheat the working fluid before the evaporator. At a heat-source temperature of 420 K, ambient temperature of 303 K and the corresponding 415 K expander inlet temperature, the thesis reports that R245fa reaches approximately 16% peak thermal efficiency in the regenerative cycle compared with approximately 14% in the basic cycle.

An important design observation is that the regenerative-efficiency curve can remain relatively flat over a broad pressure-ratio range. For R245fa, the thesis reports approximately 15% efficiency at a pressure ratio of 7 compared with a peak of about 16% at a pressure ratio of 14. This means that, within the modelled conditions, operation at a somewhat lower pressure ratio may not impose a large efficiency penalty while potentially simplifying expander design. At very high pressure ratios, the expander exhaust can become too cool for effective regeneration, producing a reduction in the benefit.

4.3 Optimum Pressure Ratio and Irreversibility

For each working fluid and expander inlet condition, an optimum pressure ratio exists. The exact optimum is dependent on whether the cycle uses a regenerator. The second-law analysis identifies the evaporator as the dominant irreversibility source. The regenerative configuration reduces this irreversibility because the preheated working fluid enters the evaporator with a smaller temperature difference relative to the heat-transfer fluid.

4.4 Scroll-Expander Semi-Empirical Results

The semi-empirical model is demonstrated using R134a, a nominal expander output of 10 kW, an orbiting speed of approximately 3000 rpm and an outlet pressure corresponding to the saturation pressure at 45°C. One representative geometry uses a base-circle radius of 4.38 mm, a scroll-wrap height of 4.1 mm and a scroll-wrap thickness of 4 mm.

The calculated expander isentropic efficiency reaches a peak for a particular pressure ratio at each inlet temperature. For the investigated cases, the efficiency remains in the approximate range of 72–76% for pressure ratios between 2.5 and 4.5. This trend is consistent with the experimental R134a scroll-expander evidence cited in the thesis, where an efficiency range of approximately 66–75% was reported over a pressure-ratio range of 2.5–5.0.

4.5 Geometric and Dimensional Findings

The Ns–Ds analysis produces a distinct domain for scroll expanders rather than overlapping directly with conventional turbomachinery. The thesis reports an Ns range of approximately 0.009–0.027 and a Ds range of approximately 10–50 for the investigated R134a database. At a fixed inlet temperature, changing aspect ratio mainly changes Ds while leaving Ns approximately constant because the thermodynamic operating conditions remain fixed.

The model indicates that a minimum volume ratio of approximately 2.1 is required to provide at least one closed chamber for the complete 360° cycle. The corresponding inlet temperature in the analysed R134a case is approximately 89°C. As inlet temperature increases to 150°C, the built-in volume ratio can rise to approximately 4.8. The study imposes an upper limit of about 5 to avoid excessive wrap turns and associated leakage.

4.6 Loss Mechanisms

The loss analysis identifies leakage as the most significant performance penalty among the principal modelled losses. Both flank and radial leakage increase with leakage gap and pressure ratio. Radial leakage is also affected by wrap perimeter, so increasing the number of turns can increase the leakage area. The thesis therefore emphasizes clearance control and appropriate volume-ratio selection as key design variables.

Mechanical losses are also important because the useful torque is the gas-force torque minus frictional losses. The model accounts for crank-pin, journal-bearing, thrust-bearing and Oldham-coupling friction. Under- and over-expansion losses arise when the actual discharge pressure does not match the condenser pressure; these losses can be reduced through appropriate built-in volume-ratio selection.

4.7 CFD Results

The CFD study is performed for a 10 kWe R134a application with expander inlet temperature varied from 100°C to 150°C, while the outlet pressure is fixed at 12.01 bar, corresponding to R134a saturation at 45°C. The two-dimensional model uses a 0.2 mm flank gap and zero radial gap.

The CFD model predicts detailed spatial and temporal behaviour that cannot be obtained from the semi-empirical lumped-parameter approach. Pressure and temperature fields evolve as the orbiting scroll changes chamber volume, while velocity contours reveal non-uniform flow structures within the expansion pockets. The mass-flux histories at the inlet and outlet are reported as nearly equal, indicating satisfactory mass conservation in the simulation.

For the simplified two-dimensional CFD case, the reported isentropic efficiency is approximately 39% for a 0.2 mm flank gap and zero radial gap when the inlet and outlet states are used as the initial and final conditions. The thesis explicitly cautions that this value should not be interpreted as the efficiency of a complete physical scroll expander because the CFD model omits mechanical components and their losses. The CFD result is therefore more useful for qualitative

and comparative analysis, including leakage-flow behaviour, transient pressure development and torque periodicity.

4.8 Semi-Empirical Model versus CFD

Aspect	Semi-Empirical Model	CFD Model
Computational cost	Low; suitable for rapid iterations	High; transient dynamic mesh
Geometry treatment	Lumped chamber geometry	Spatially resolved moving domain
Outlet-state prediction	Primary strength	Available with detailed field information
Pressure/temperature field	Not spatially resolved	Spatially resolved
Leakage	Empirical/analytical model	Resolved through CFD gap flow within model limits
Mechanical losses	Included in semi-empirical formulation	Not included in simplified CFD case
Design role	Initial design and optimization	Fine-tuning and qualitative physics
Dimensional analysis	Directly integrated with Ns - Ds study	Primarily used for detailed field interpretation

Table 3. Methodological comparison based on the modelling conclusions of the uploaded thesis.

5. Key Findings and Engineering Implications

- Moderate-temperature micro-solar thermal generation requires a cycle better matched to low-grade heat than a conventional small steam Rankine system.
- Organic fluids with dry or approximately isentropic expansion behaviour are better aligned with the investigated application than water.
- R245fa and R134a are identified in the thesis as strong candidates for further scroll-expander investigation.
- Regeneration improves cycle thermal efficiency by recovering useful heat from the expander exhaust; for the reported R245fa case, peak efficiency rises from about 14% to about 16%.
- An optimum pressure ratio exists for each working fluid and inlet condition, and the optimum changes when regeneration is introduced.
- The evaporator is the dominant source of irreversibility in both basic and regenerative ORC configurations.
- For scroll design, specific-volume ratio, pressure ratio, pressure difference, p - v behaviour and sound-speed variation are important thermodynamic inputs.
- A specific-volume ratio threshold of about 20 is suggested during thermodynamic screening, while the R134a scroll database uses a built-in volume-ratio upper limit of about 5 to limit wrap complexity.

- Semi-empirical scroll modelling is suitable for rapid prototyping because it requires comparatively little computational effort.
- Leakage is identified as the most significant scroll-expander loss mechanism in the investigated loss analysis.
- The Ns–Ds approach provides a non-dimensional framework for representing scroll-expander geometries and indicates a distinct operating domain.
- CFD is valuable for resolving transient flow and thermal fields, but the two-dimensional simplified model should not be treated as a complete prediction of physical expander efficiency.

6. Limitations of the Present Study

The findings are subject to the assumptions and modelling choices in the source thesis. The ORC analysis uses prescribed component efficiencies and simplified heat-exchanger pressure-drop and pinch assumptions. The detailed scroll-expander analysis is primarily demonstrated for R134a, so the geometric conclusions are not automatically transferable to every working fluid. The CFD study is two-dimensional and does not include the full mechanical assembly, which explains why its predicted performance can differ substantially from the semi-empirical result and from an actual device.

The thesis also notes that currently available CFD software is not straightforward to adapt to scroll geometry because the computational domain changes at every time step. Furthermore, the role of oil in oil-flooded scroll machines remains insufficiently understood in the modelling framework. These limitations should be considered when interpreting the results and when extending the work to practical prototype design.

7. Conclusions

This research establishes a linked thermodynamic and computational framework for evaluating scroll expanders in micro-solar ORC systems. The work begins with the recognition that moderate-temperature solar heat is difficult to convert efficiently using small steam Rankine systems. ORC provides a more compatible cycle architecture because the working fluid can be selected to match the heat-source temperature and to avoid wet expansion.

The thermodynamic analysis demonstrates that working-fluid properties strongly influence pressure ratio, volume ratio, enthalpy drop and the geometry required for the expander. R134a and R245fa emerge as important candidates for the detailed expander study. Regeneration improves cycle efficiency and reduces evaporator irreversibility by recovering heat from the expander exhaust. However, the benefit of regeneration depends on pressure ratio because the exhaust temperature must remain sufficiently high for useful heat recovery.

The semi-empirical scroll model provides a practical design tool. For the investigated R134a case, the model predicts approximately 72–76% isentropic efficiency across a pressure-ratio range of 2.5–4.5. The dimensional-analysis study shows that scroll expanders occupy a distinct

Ns–Ds domain and that aspect ratio can be used to generate alternative geometries for a fixed thermodynamic operating point. The loss analysis identifies leakage as a major design concern, making clearance control, wrap geometry and volume-ratio selection central to performance optimization.

The CFD investigation complements the semi-empirical approach by providing spatial information on the transient flow and thermal fields. The nearly equal inlet and outlet mass fluxes support the conservation behaviour of the numerical solution, while the periodic torque response provides information relevant to mechanical-system design. The reported two-dimensional CFD efficiency of approximately 39% should be interpreted only within the simplified CFD model because mechanical losses and other physical components are omitted.

Overall, the research supports a sequential design methodology: use thermodynamic analysis to select the working fluid and operating point; use semi-empirical modelling for rapid scroll-geometry screening and optimization; and use CFD to examine local flow physics, leakage and transient effects before proceeding to experimental validation and three-dimensional design.

8. Recommendations for Future Research

- Extend the fluid study from pure working fluids to zeotropic and other ORC mixtures to investigate reduced heat-exchanger irreversibility.
- Develop equivalent Ns–Ds-based design methodologies for screw and rotary-vane expanders for direct comparison with scroll machines.
- Develop a fully three-dimensional transient CFD model capable of resolving inlet, outlet and internal vortex structures.
- Include the complete mechanical assembly and bearing/friction losses in high-fidelity numerical models.
- Develop improved leakage correlations using combined CFD and experimental data, particularly outside conventional clearance ranges.
- Investigate oil-flooded and two-phase leakage behaviour, which remains an open modelling problem.
- Perform experimental validation of optimized scroll geometries under the same pressure ratios and temperature ranges used in the numerical work.
- Carry out coupled thermo-mechanical analysis to verify scroll-wrap structural stability under pressure differences between adjacent chambers.
- Revisit the ORC cycle optimization iteratively with the actual predicted scroll-expander efficiency rather than prescribing a constant expander efficiency.
- Assess techno-economic performance and levelized cost of electricity for a complete micro-solar ORC installation.

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