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Developing a Framework for Modelling and Analysing of Multi-Stage Screw Compressors



By

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Thesis submitted for the degree of Doctor of Philosophy
in Mechanical Engineering

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May 2025

*I dedicate this thesis to my beloved mother,
who became my guiding light after my father's passing
at a young age. Her unwavering strength, wisdom,
and unconditional love have been the foundation of my journey.
For everything I have achieved, I owe it to her.*

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Abhishek Kumar

London, 19th May 2025

Declaration

I confirm that this work is my own except where indicated by reference in the text. I agree for this work to be submitted to the Institutional Repository of City St George's, University of London for use in accordance with the Thesis Deposit Agreement and the agreement between Kirloskar Pneumatic Company Limited and City St George's, University of London over confidentiality of the intellectual property, which are outcomes of their joint collaborative project.

Abhishek Kumar

London, 19th May 2025

Abstract

Screw compressors are widely used in industries such as manufacturing, energy, and construction, contributing significantly to industrial electricity consumption. Despite the growing market, projected to reach \$19.37 billion by 2030 at a CAGR of 6.5%, multi-stage screw compressors face operational challenges, including rotor deformation, limited bearing life, ineffective cooling, and condensate dropout in high-pressure applications. This research addresses these challenges by developing a comprehensive modelling framework to enhance the performance and economic viability of multi-stage screw compressors.

The proposed framework integrates a conventional chamber model with machine learning techniques to perform thermodynamic analysis and optimisation. Key parameters such as profile clearances, rotor geometry, and fluid injection are optimised for both individual and final stages using evolutionary and probabilistic methods, achieving high accuracy while reducing computational costs. Experimental validation was conducted on a prototype two-stage oil-flooded air screw compressor for water-well applications, demonstrating the reliability of the model.

In addition to performance optimisation, this study presents an extensive economic analysis comparing single-stage and multi-stage compressors for power ranges of 22–315 kW and delivery pressures of 6–12 bar. A cost-effective design incorporating advanced rotor profiles and optimised sealing and cooling systems was developed. Over a 10-year lifecycle, the two-stage compressor showed a 20–75% reduction in operational costs, significantly lowering life-cycle expenses compared to its single-stage counterpart.

This research contributes to screw compressor technology by addressing the limitations of multi-staging, providing a proven modelling and optimisation methodology, and demonstrating the economic benefits of multi-stage systems for industrial applications.

List of Symbols

Abbreviations	
AC	Alternating Current
ANN	Artificial Neural Network
CFD	Computational Fluid Dynamics
DC	Direct Current
DES	Detached Eddy Simulation
ETAK	Adiabatic Efficiency
ETAV	Volumetric Efficiency
GA	Genetic Algorithm
GPR	Gaussian Process Regression
GUI	Graphical User Interface
HP	High Pressure
LP	Low Pressure
ML	Machine Learning
RMSE	Root Mean Squared Error
SCORG	Screw Compressor Rotor Grid Generation
SVM	Support Vector Machine
VI	Built-in Volume Ratio
RPM	Rotations Per Minute

Roman Symbols

A	Flow area (m ²)
A_k	Total effective area of clearance (m ²)
A_t	Blade throat area (m ²)
C_{initial}	Initial capital cost
$C_{\text{operating}}$	Operating cost
$C_{\text{lifecycle}}$	Lifecycle cost
D_{oil}	Oil port diameter (mm)
D_{male}	Male rotor outer diameter (mm)
F_{IOIL}	Oil injection angle (°)
GAP_A	Axial clearance (mm)
GAP_I	Interlobe clearance (mm)
GAP_R	Radial clearance (mm)
H	Total operating hours
L/D	Relative length of rotors
M	Mass (kg)
N	Speed (rpm)
P	Power consumption (kW)
P_{dis}	Discharge pressure (bar)
P_{suc}	Suction pressure (bar)
P_{oil}	Oil injection pressure (bar)
P_a	Adiabatic power (kW)
P_{in}	Suction pressure (bar)
P_1	Interstage pressure (bar)
Q	Volume flow rate (m ³ /min)
R^2	Coefficient of determination
SPC	Specific power consumption (kW/m ³ /min)
T	Temperature (°C)
T_{suc}	Suction temperature (°C)
T_{oil}	Oil injection temperature (°C)
V_s	Suction volume (mm ³)
V_d	Discharge volume (mm ³)
$V_{\text{theoretical}}$	Theoretical volume (mm ³)
W_{tip}	Tip speed of the male rotor (m/s)
$\dot{m}$	Mass flow rate (kg/s)

η_{ad}	Adiabatic efficiency (%)
η_{vol}	Volumetric efficiency (%)
ϕ	Wrap angle (°)
ρ	Density (kg/m ³)
δ	Female rotor deflection (mm)
ζ	Leakage flow resistance coefficient
θ	Oil injection angle (°)
γ	Adiabatic constant
h_{in}	Fluid enthalpy (inflow)
h_{out}	Fluid enthalpy (outflow)
v	Fluid velocity (m/s)

Chapter 1

Introduction

1.1 Background

In recent decades, the utilisation of compressed air has become widely recognised. It is utilised as an energy source and as active air. It serves as an energy source for operating pneumatic machinery; when this compressed air directly contacts the product, it is referred to as active air. The utilisation of compressed air encompasses all manufacturing processes, including aerospace, automotive, chemical, electronics, food and beverage, glass production, and medicines. Understanding the production of compressed air is critical due to its significance. This study examines a positive rotary twin screw machine designed for high-pressure applications.

Rotary Twin Screw Compressors have been utilised in industry for an extended period, with its initial proposal occurring in 1878 by Heinrich Krigar in Germany ([1]). Their advancement as compressors or expanders was constrained by their low efficiency and elevated production costs. The asymmetric rotor profile, created in 1973 ([1]), markedly lowered leakage via the blow hole. The advent of CNC machine tools enabled the production of helical rotors featuring intricate features. Contemporary screw machines are considered exceptionally reliable and compact technologies for energy conversion. This is typically favoured for comparatively low discharge pressure and a broad spectrum of flow rates over reciprocating, centrifugal, and axial compressors. It is a compact, dependable, and economical apparatus comprising a pair of helical rotors with four to six bearings encased within a housing. It has been classified as an oil-flooded, oil-free, and water-injected screw compressor. The oil-flooded variant dominates the market share because to its reduced mechanical components, enhanced efficiency, and capability to attain elevated pressure in a single stage. Screw compressors have undergone constant enhancements owing to its straightforward design and dependability, thereby reducing internal leakage, friction losses between the rotors, and augmenting flow capacity. There remains significant potential for tweaking parameters to improve screw compressor performance.

1.2 Motivation

Compressed air systems are essential in various industries, such as manufacturing, construction, and energy, constituting roughly 10-20% of overall industrial electricity usage [2]. Screw compressors are integral to these systems; yet, their enormous energy requirements significantly contribute to global carbon emissions. Given the increasing environmental concerns, enhancing the energy efficiency of screw compressors is essential [3, 4]. Statistical data from KPCL indicate that approximately 68% of the life-cycle cost of a screw compressor is ascribed to operational expenses, predominantly resulting from power consumption (see figure 1.1). This underscores the necessity of prioritising power reduction or enhancing compressor efficiency, as even marginal improvements can yield substantial energy savings and environmental advantages. Optimising screw compressor parameters is crucial for improving performance and minimising power usage, hence rendering these devices more environmentally friendly.

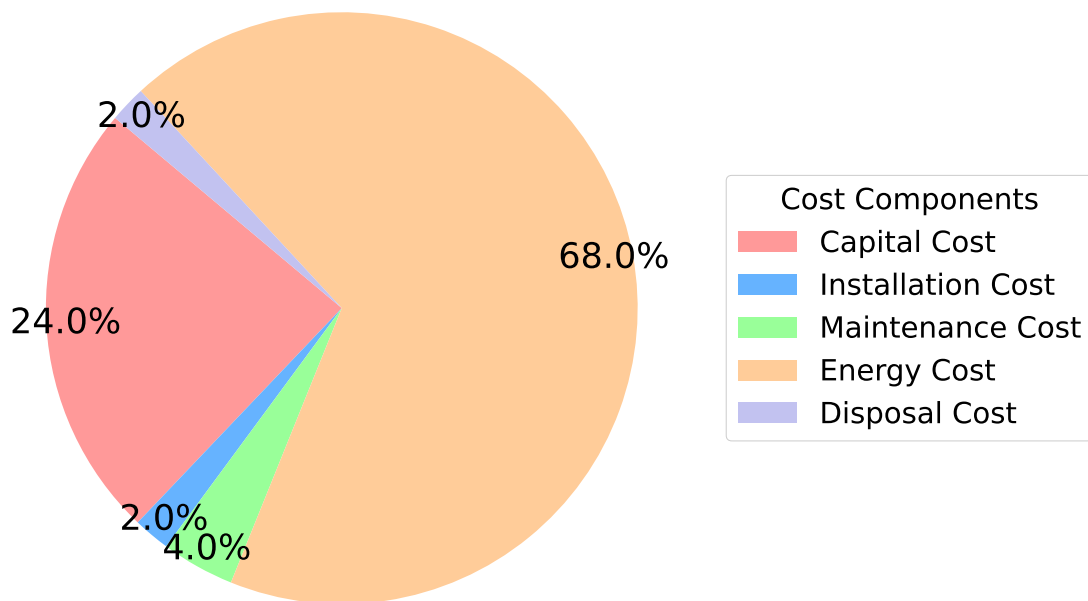


Figure 1.1: Lifecycle cost distribution of a typical single-stage oil-flooded air screw compressor system with a 22 kW power rating and an 8.5 pressure ratio over a 10-year period [5].

The global air compressor market is projected to develop at a compound annual growth rate (CAGR) of 3.5% by 2030 (Refer to figure-1.2 [6], while the screw compressor sector is anticipated to grow at a more rapid rate of 6.5%, with a market value of around \$19.37 bil-

lion [7]. Notwithstanding this expansion, multi-stage screw compressors remain infrequently utilised, particularly in applications over 30 bar, owing to issues such as rotor bending deformation, constrained bearing longevity, and insufficient cooling from injected oil [8]. In the lower pressure range, screw compressors are not preferred for multi-stage applications, which are mostly led by reciprocating compressors that provide superior pressure capabilities. These

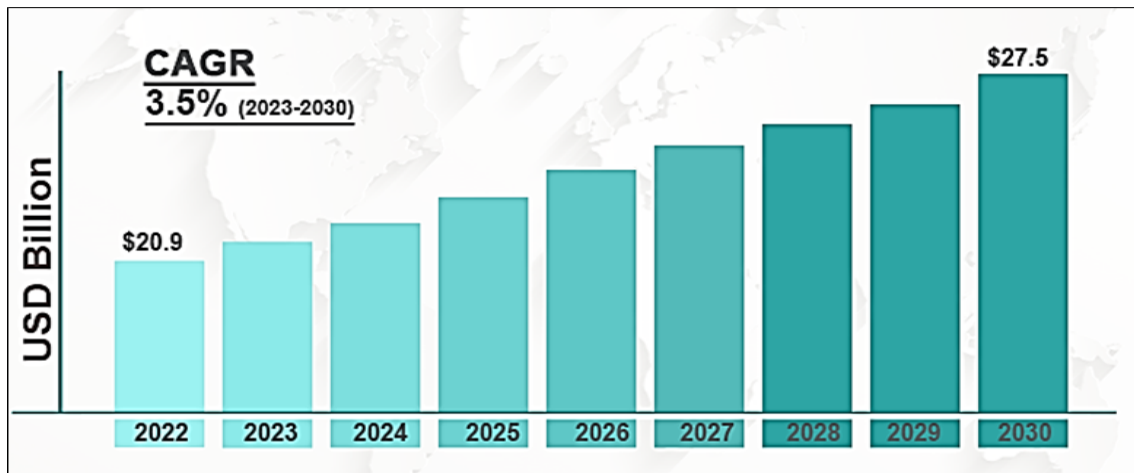


Figure 1.2: Global air compressor market share is expected to grow at a CAGR Of 3.5% by 2030 [6, 7].

problems highlight the necessity for novel research and innovation. The opportunity to improve the efficiency of screw compressors by adjusting critical parameters—such as rotor geometry, profile clearances, and fluid injection—remains significantly underutilised. Addressing the obstacles currently obstructing the widespread implementation of multi-stage screw compressors can provide substantial enhancements in energy efficiency and operational effectiveness.

This study aims to create an improved optimising and modelling framework for multi-stage screw compressors. This system seeks to properly forecast and improve compressor performance and reduce power consumption by mixing traditional chamber models with machine learning approaches. The primary objective is to provide a tested and economically feasible solution that minimises the operational expenses of screw compressors, while also advancing global sustainability by decreasing energy consumption and carbon emissions.

1.3 The twin screw compressor

The twin screw compressor is a positive displacement apparatus, extensively utilised in industrial applications owing to its dependability, efficiency, and capacity to manage elevated pressure ratios. It comprises two interlocking helical screw rotors, known as the male and female

rotors, contained within a compression chamber. The rotors are the sole moving components of the compressor, engineered with integrated shafts that accommodate drive mechanisms, bearings, and seals. The male rotor often possesses fewer, thicker lobes, whereas the female rotor features a greater number of thinner grooves, facilitating accurate meshing during operation [1].

As the rotors spin, a designated volume of air or gas is sucked into the compressor's inlet and confined within the cavities created between the lobes of the two rotors. As rotation persists, the confined volume translocates longitudinally down the rotor axis, progressively diminishing the space occupied by the gas. The decrease in volume results in an increase in gas pressure, a phenomenon referred to as compression. Upon reaching the requisite pressure, the compressed gas is expelled from the outlet port.

A primary advantage of the twin screw compressor is its capacity to attain elevated rotational speeds owing to the balanced rotary motion of the intermeshing rotors. This innovation enhances power density and improves overall efficiency by reducing mechanical vibrations and facilitating smoother operation. Moreover, the lack of reciprocating components diminishes wear and tear, leading to an extended service life and reduced maintenance expenses in comparison to other compressor varieties, such as reciprocating compressors.

In oil-injected twin screw compressors, lubricating oil is fed into the compression chamber to seal gaps, minimise mechanical losses, and assist with heat dissipation. This enhances volumetric efficiency by mitigating leakage between the rotors and augmenting the overall cooling effect. Nevertheless, the oil must be extracted from the compressed gas prior to its escape from the system, necessitating further filtration apparatus.

Dry twin screw compressors, conversely, operate without oil throughout the compression process and are optimal for applications necessitating oil-free air or gas, such as in the pharmaceutical or food sectors. In these systems, efficiency depends exclusively on the accuracy of rotor design and the tightness of clearances, requiring sophisticated manufacturing methods.

The design of the twin screw compressor enables scalability, rendering it appropriate for various pressures and flow rates. Although its application is typically restricted to single-stage configurations for lower pressures, multi-stage configurations may be employed for greater pressures; however, they are less prevalent due to issues related to rotor deformation, bearing wear, and thermal management.

In summary, the twin screw compressor's straightforward yet durable design, including

two interlocking rotors, allows for efficient operation at elevated speeds and pressures. Its adaptability, together with its capacity to manage diverse gases and operating situations, renders it a favoured option in sectors such as manufacturing, energy, refrigeration, and air conditioning.

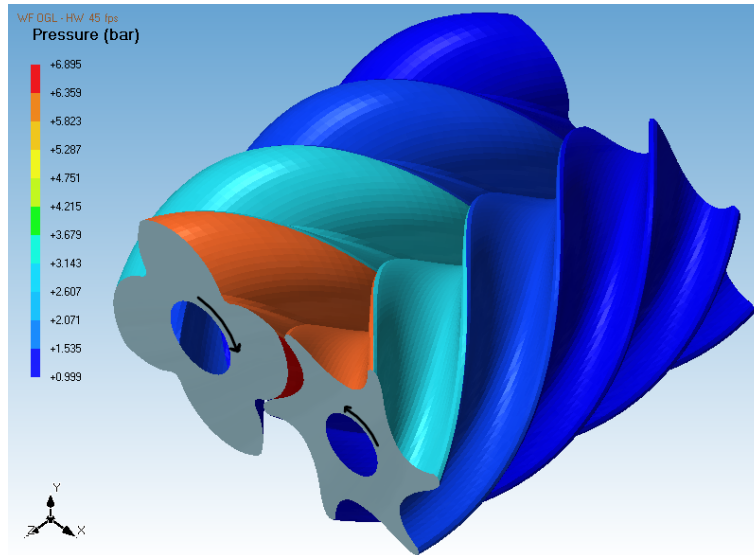


Figure 1.3: Illustration of the working principle of a screw compressor, showing the pressure distribution across the rotor lobes during compression [9].

1.4 High-pressure applications

High-pressure compressed fluid is essential in various industries, including oil and gas, pipeline services, offshore exploration, well drilling, and plastics manufacturing. Certain applications, such the initiation of air compressors for big diesel engines and fuel gas boosters, necessitate dependable high-pressure compression systems (see figure-1.4). These industrial industries generally necessitate discharge pressures of 40 bar or more for optimal performance.

Reciprocating compressors are typically preferred for pressures above 40 bar because of their ability to manage high compression ratios within a compact design. They are extensively utilised in high-pressure applications due to their durable design and capacity to successfully handle variable demand and pressure surges. Multi-stage screw compressors have become increasingly popular for applications necessitating pressures up to 40 bar, owing to their superior efficiency, reliability, and capability for continuous operation with minimal maintenance.

Multi-stage screw compressors provide an efficient solution for applications requiring el-

evated flow rates and moderate pressures, including gas compression, refrigeration, and chemical processing. The capacity to manage several compression stages inside one machine enhances energy consumption control, hence dramatically lowering operational costs compared to single-stage systems. Notwithstanding their benefits, multi-stage screw compressors have historically been underutilised for pressures over 30-40 bar, mostly due to issues such as rotor deformation, bearing longevity, and thermal regulation.

For elevated discharge pressures, compound compressors, which integrate a single-stage screw compressor with a multi-stage reciprocating compressor, are frequently utilised. These hybrid systems utilise the superior volumetric efficiency of screw compressors for initial compression stages, while the reciprocating compressor manages the latter compression stages, attaining the requisite pressure levels with enhanced overall efficiency (Refer-[8]). This method is especially beneficial in scenarios necessitating both elevated flow rates and high discharge pressures, providing a cost-effective and energy-efficient alternative.

With the rising need for high-pressure systems, especially in the oil and gas sectors, the necessity for creative solutions to enhance the performance of multi-stage screw compressors is becoming paramount. This research seeks to create an innovative modelling and optimisation method to improve the efficiency of multi-stage screw compressors, hence increasing their suitability for high-pressure applications. The research aims to enhance key parameters, including rotor geometry, fluid injection, and profile clearances, to align current multi-stage systems with the requirements of high-pressure industrial applications, illustrating the potential for screw compressors to assume a more significant role in these fields.

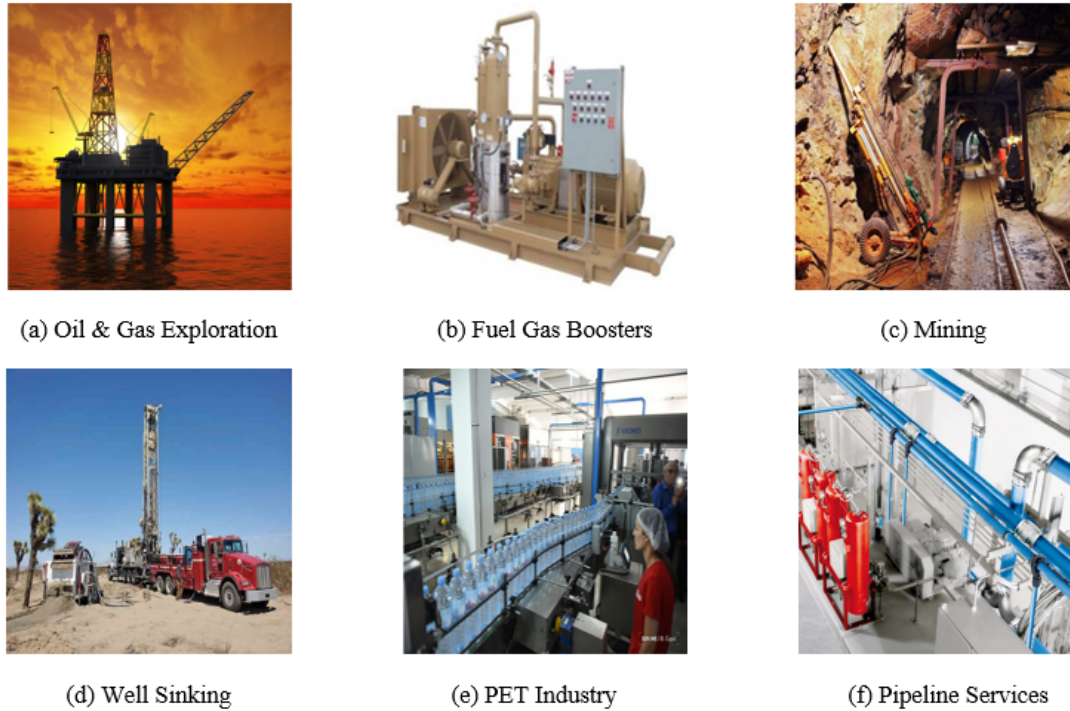


Figure 1.4: Application of high-pressure compressed fluid

1.5 Implementation of Artificial Intelligence in screw compressors

In recent years, the utilisation of Artificial Intelligence (AI) in engineering systems has surfaced as a revolutionary method, providing significant potential for performance improvement, design optimisation, and operational efficacy. The global AI market, estimated at around USD 638.23 billion in 2024, is anticipated to attain USD 3680.47 billion by 2034, exhibiting a compound yearly growth rate (CAGR) of 19.1% from 2024 to 2034 [10]. This exponential rise signifies AI's increasing influence in transforming industrial processes across multiple sectors.

AI enables the automation of monotonous and time-intensive operations, allowing engineers to concentrate on intricate problem-solving, creativity, and strategic decision-making. In the domain of screw compressors, artificial intelligence presents substantial prospects for tackling critical issues of performance forecasting, design enhancement, and system dependability. AI approaches can be employed for rotor profile development, efficiency prediction, parameter optimisation, predictive maintenance, problem identification, and inventory management.

The amalgamation of AI techniques, especially Machine Learning (ML), with traditional

screw compressor systems facilitates the modelling of intricate, non-linear correlations between input variables and performance outcomes. This feature improves forecasting precision and facilitates the formulation of data-driven optimisation strategies. Methods including Gaussian Process Regression (GPR), Artificial Neural Networks (ANNs), and various probabilistic models enable the determination of optimal design parameters, enhance energy efficiency, and decrease operational expenses.

This study examines the application of AI for performance forecasting and parametric optimisation of single-stage and multi-stage screw compressors. The research emphasises the utilisation of evolutionary algorithms, including Genetic Algorithms, in conjunction with probabilistic optimisation techniques such as Bayesian optimisation, to improve compressor efficiency. This study utilises AI-driven methodologies to overcome the constraints of conventional modelling techniques, providing a comprehensive framework for the design, analysis, and optimisation of screw compressors across many industrial applications.

1.6 Summary

This chapter has presented a comprehensive overview of twin screw compressor technology, emphasizing its pivotal role in industrial applications and the growing importance of energy efficiency. It traced the historical evolution of screw compressors, described their operating principles, and highlighted challenges specific to multi-stage and high-pressure applications, such as rotor deformation, bearing wear, and thermal limitations. The chapter also discussed key industry trends, including the rising demand for high-efficiency compressors and the expanding market potential.

Furthermore, the relevance of Artificial Intelligence (AI) in modern engineering systems was introduced, particularly its emerging applications in the screw compressor domain. The chapter outlined how AI, and more specifically Machine Learning techniques, can aid in performance prediction, design optimisation, and system reliability improvements.

This foundational discussion sets the stage for the subsequent chapters. The next chapter offers a detailed literature review, identifying key research developments, knowledge gaps, and how the present work contributes to advancing screw compressor modelling and optimisation frameworks.

Chapter 2

Literature Review

The literature review is structured into three primary sections: the first presents a chronological examination of all pertinent literature, while the second provides an in-depth analysis of the optimisation techniques employed in screw compressor designs and profile generation to enhance efficiency. The final section examines the existing literature on high-pressure applications and identifies the gaps therein. It provides a framework for developing a multi-stage screw compressor and addresses the disparity between current optimisation strategies for enhancing multi-stage parameters and boosting machine performance.

2.1 General review

A screw compressor, or twin screw compressor, is a positive displacement rotary compressor that operates efficiently at high speeds throughout a broad spectrum of pressures and flow rates. They function as both compressors and expanders. These rotary machines are typically employed to provide compressed air in the construction, food processing, textiles, chemicals, and pharmaceutical sectors. Their design is uncomplicated, including moving components that comprise merely two rotors revolving within four to six bearings. Owing to their exceptional reliability, little initial cost, lightweight construction, reduced maintenance requirements, and compact design, they constitute a significant share of all positive displacement compressors sold and in operation. They function with a diverse array of working fluids, including gases, dry vapours, or multiphase mixtures, with phase transitions occurring within the apparatus. Their operational method may involve the absence of internal lubrication, oil flooding, or the injection of other fluids during the compression or expansion phases. In this book [1], the author discusses the subsequent aspects:

- The volumetric changes occurring in screw compressors transpire in three dimensions rather than two.
- Each chamber has a discernible starting point where the initial trapped volume is zero. As rotation progresses in the direction indicated by the arrows, the trapped volume grows

as the line of contact between the rotors advances along the axis towards the rear.

- Consequently, during a full revolution (360 degrees) of the main rotor, the trapped volume within the chamber reaches its maximum, extending in a helical configuration nearly throughout the whole length of the rotor.
- Subsequent rotation results in the chamber being severed from the port, leading to a gradual decrease in volume that induces axial and bending stresses on the rotors, as well as contact forces between the rotor lobes.
- An efficient screw compressor must possess a profile characterised by a substantial flow cross-sectional area, a brief sealing line, and a minimal blow hole area.

It discusses the geometry and profile of the screw compressor and the impact of each parameter on its performance. The thermodynamic performance is assessed via the multi-chamber model, employing the mass continuity and energy conservation equations. The derived differential is subsequently solved numerically utilising the Runge-Kutta technique, which converges to optimal results and yields the values of temperature and pressure. Utilising the ideal gas law, the remaining unknown variables can be determined. This book serves as a comprehensive guide to screw compressors, including an overview of their operation and applications. In the papers [11] and [12], the authors present a methodology for the construction of screw compressors and expanders, which is predicated on a distinct algorithm for determining rotor profiles and a model for fluid dynamics and thermodynamic processes within the machinery. Part I of the study delineates the algorithm for profiling the screw rotor. It demonstrates a condition of conjugacy, which, when addressed, permits the delineation of several essential arcs through the analysis or manipulation of distinct points. The implementation renders the design significantly more manageable, requiring simply the specification of major arcs. These may be located on the main or gate ridge, or on any other rotor connecting rack, which serves as a non-rotating radiator. The subsequent arcs are then created automatically from this. Thus, any amalgamation of profiles may be contemplated. The optimal performance has been attained in the integrated rotor-rack production process. This combination yields a rotor profile featuring a more robust lobe and superior output compared to all other known types. Part II delineates a mathematical model for the compression and expansion processes in precisely calibrated compactors, which are thoroughly described about their compressor design and the associated screws and extensions.

According to Stosic et al.[13]: The escalating needs of functional screw compressors necessitate that compressor designs be consistently aligned with their operational, energetic,

and productive capacities. This document outlines the correct methodology for optimising the shape, dimensions, and operational characteristics of a screw compressor, resulting in the best suitable design for a specific compressor function. The algorithm for generating rack profile rotors is integrated with a numerical model of compressor fluid dynamics and thermodynamic processes. Compressors are engineered to achieve superior delivery rates, and their performance surpasses that of conventional methods. Additional individuals The challenges associated with improving the rotor profile and compressor components are examined, utilising a 5/6 lobe configuration and a 106 mm screw compressor to substantiate the findings. The top rotor profile, compressor speed, oil flow rate, and temperature exhibit significant variation when compressed with different gases or vapours.

According to Kovacevic et al.[14]: The author emphasises the utilisation of natural refrigerants, such as CO₂, as alternatives to halogenated hydrocarbons due to their absence of ozone-depleting effects. The primary issue related with utilising CO₂ as a refrigerant is the substantial pressure differentials across the compressor and the considerable efficiency losses linked to the throttling process within the refrigeration cycle. The author introduces an innovative technique employing a screw machine to compress gas and harness power during the expansion phase. The notable aspect was that a single set of rotors was employed for both the compressor and expander, in a design that partially mitigates the forces generated by the pressure differential, hence decreasing the bearing loads to an acceptable threshold.

According to Madhav et al.[15]: The increasing demand for oil-free compressed air in sectors such as food and drinks, chemicals, textiles, pharmaceuticals, and automotive fuel cells necessitates class-0 air quality. The water-injected method use water for injection between the rotors, offering certain advantages over oil-injected and oil-free screw compressors, as detailed below:

- The specific heat of water is greater than specific heat of oil which means quantity of water to be injected is lower compared to oil.
- The viscosity of water is less than viscosity of oil that yields in lower viscous drag. Hence, frictional power loss will be lower.
- Water injected screw compressor can run at temperature even below the dew point as there is no issues associated with condensation.
- As oil is not used so less chance of fire accidents.
- Near isothermal compression.

This literature clearly indicates that the specific power consumptions are 8% and 18% lower than those of oil-injected and oil-free screw compressors, respectively. The life-cycle costs are 7% and 25% lower than those of oil-injected and oil-free machines, respectively. The technical hurdles encountered include:

- Scaling corrosion of materials.
- Poor lubricity of water.
- Selection of rotor material.
- Bearings selection.
- Poor sealing.
- Bacterial pollution due to presence of water.

According to Yan et al.[16]: The term plastic, originally signifying malleable and easily moulded, has recently come to denote a category of materials known as polymers. They consist of elongated, repetitive chains of molecules whose distinct properties are mostly determined by the kind of molecules involved and their bonding arrangements. The synthesis of polymers from monomers is termed polymerisation. Polymers are fundamentally classified into two categories: synthetic and natural. They are observable in nearly all daily activities, from consuming water bottles to utilising modern devices. They are extensively utilised in the aerospace sector, optical engineering, and biomaterials owing to their superior attributes, including low density, corrosion resistance, low friction coefficient, and potential for mass production. In this transformative era of polymers, thermoplastic polymers have provided a competitive advantage in the manufacturing sector. During a recent virtual conference at City University, in collaboration with VICTREX and HOWDEN, the thermoplastic polymer PEEK (Poly ether ether ketone) was addressed, highlighting its excellent mechanical strength and potential uses in compressor technology.

This article demonstrates that oil injection substantially enhances the performance of an oil-flooded screw compressor [4]. The effect is contingent upon the mass flow rate of the working fluid, the shaft speed, the injection location, and the temperature of the injected oil. Tests have been conducted on an air compressor featuring a male rotor diameter of 98 mm, equipped with injection nozzles measuring 2, 3, and 4 mm, as well as a nozzle with numerous apertures. The trials were conducted at discharge pressures of 6.5, 8.5, 10.5, and 12.5 bar, with

rotor speeds of 3000, 4000, and 5000 rpm. Consequently, it is noted that fluctuations in oil volume flow rate exert a significantly greater influence on power consumption than air flow rate, given a constant discharge pressure and male rotor shaft speed. At reduced discharge pressures, power consumption escalates with the augmentation of oil flow. Therefore, an optimal quantity of oil must be established for a compressor operating under defined design conditions.

2.2 Optimisation techniques applied to the design of a twin-screw

The rising demand for more efficient screw compressors has propelled substantial developments in the design and optimisation of these machines. Compressor designs are customised to fulfil particular specifications based on operational conditions, including capacity, duty cycles, and manufacturing limitations. The optimisation of a twin-screw compressor entails enhancing its geometry, dimensions, and operational characteristics to get the best suitable design for a specific application or working fluid.

Numerous research in the literature demonstrate diverse optimisation approaches employed in screw compressors. For example, [17] presented an optimisation method for a refrigeration twin-screw compressor, emphasising rotor geometric parameters including wrap angle, relative length (length-to-diameter ratio), and sliding valve configurations. These characteristics are essential for compressor efficiency and for minimising female rotor deflection, bearing loads, and rotor contact forces. Likewise, [18] examined the optimisation of lobe combinations, relative length, and wrap angle, all of which influence compressor performance. [11] introduced a methodology for rotor profile generation utilising conjugacy conditions, facilitating the development of highly efficient rotor profiles via the selection of primary arcs.

Evolutionary optimisation strategies have been investigated, particularly by [19, 20], who utilised Evolution Strategy (ES) for the optimisation of screw compressors. The research emphasised the constraints of penalty function methodologies and proposed an enhanced offspring generation strategy to tackle the issues of global and local optima.

Genetic Algorithms (GA) are extensively utilised among optimisation strategies due to their requirement for only the goal function's value and their capability to manage discontinuous functions. Nonetheless, genetic algorithms often exhibit sluggish convergence rates because to their limited population size. Furthermore, the box complex method, as illustrated by [13], is a frequently employed technique. It necessitates solely function values and does not require gradients; nonetheless, it is less appropriate for issues involving discrete parameters.

The optimisation of intricate geometries, such as those associated with screw compressors, has been enhanced by advanced techniques like NURBS (Non-Uniform Rational B-Splines), as detailed by [21], facilitating more precise control over complex shapes.

Subsequent research by [22] utilised a chamber model generator and simulation tools to improve rotor profiles while reducing energy expenses. This methodology has been empirically validated. Structural optimisation has been implemented in twin-screw expanders, as demonstrated by [23], who investigated the impact of geometric parameters on thermal performance and leakage effects utilising a sequential quadratic programming approach.

Moreover, various other studies examine optimisation methods in analogous domains, including centrifugal compressors and heat pumps. For example, [24] demonstrated the design optimisation of a centrifugal compressor impeller utilising a Radial Basis Neural Network, enhancing isentropic efficiency by 1%. Simultaneously, [25] presented an automated design framework utilising multi-objective optimisation and Artificial Neural Networks (ANN), attaining a four-order magnitude acceleration relative to traditional 1D radial modelling of turbocompressors.

Screw compressors possess essential operating parameters including volume output, efficiency, specific power needs, wrap angle, and length-to-diameter ratio [26, 17, 27]. These parameters are significantly influenced by the shape of the flow-through section, affecting both volumetric efficiency and specific performance [22]. Optimising these geometric parameters is crucial for enhancing screw compressor performance [26]. Specifically, the selection of rational geometry necessitates intricate optimisation methods and mathematical models.

The creation of composite screw rotors via Resin Transfer Moulding (RTM) techniques can decrease manufacturing costs and rotor weight, as evidenced by [28, 29]. Composite screw rotors fabricated from chopped carbon fibre epoxy using RTM demonstrated a 52% reduction in weight compared to aluminium rotors.

There have been considerable breakthroughs in the optimising of rotor lobe profiles. [30] delineated novel lobe profiles that enhance delivery rates and reduce leaks, whereas [18] examined the impact of rotor geometry, encompassing wrap angles and lobe configurations. These research determined the ideal rotor geometries for several applications:

- 4+5 combination: Suitable for light, low-pressure applications.
- 5+6 combination: Ideal for high efficiency, though it may face challenges at high pres-

sures.

- 5+7 combination: Best for high length-to-diameter ratios and high-pressure operations.
- 4+6 combination: Lower efficiency but versatile across different parameters.

Subsequent optimisation study by [31] concentrated on identifying inter-rotor clearances and their effect on leakage rates, demonstrating that improved clearance distributions enhance thermodynamic performance. Research by [32] improved rotor profiles for twin-screw compressors, highlighting scoop area, polar moment of inertia, and blowhole height as essential criteria for enhancing performance.

The efficacy of oil-injected screw compressors has been another focal point of examination. Fujiwara (1995) suggested a novel rotor profile for oil-injected screw compressors, exhibiting remarkable concordance between experimental and projected efficiency [33]. Furthermore, [21] employed NURBS to optimise screw compressor rotor profiles, providing enhanced performance and adaptability relative to conventional Bezier representations.

Massoudi et al. (2022) presented an automated design framework employing multi-objective optimisation and artificial neural network models to assess robustness and optimise mass-flow ranges, resulting in a substantial acceleration of design optimisation procedures [25]. Alternative optimisation tools, such the SUMT method introduced by [34], improved twin-screw rotor performance by explicitly improving rack design and preventing undercutting.

Comprehensive studies on rotor optimisation underscore the pivotal role of geometrical parameters in influencing compressor performance. These optimisation strategies result in enhanced energy efficiency, diminished maintenance expenses, and extended machine longevity, fostering the advancement of more sustainable and economically viable screw compressors.

2.3 An analysis of high-pressure screw compressors

From a thermodynamic standpoint, multi-stage compression with interstage cooling offers considerable energy savings relative to single-stage compression. This technique is extensively utilised in applications requiring high-pressure ratios, particularly in the oil and gas, pipeline services, offshore exploration, and fuel gas booster industries, where high-pressure compressed fluids are essential. Single-stage screw compressors are limited to pressures below 18 bar, requiring multi-stage setups to attain higher pressure outputs. Figure 2.1 illustrates the P-V di-

agram for a two-stage compressor, highlighting the advantages of multi-staging in enhancing compressor efficiency and performance.

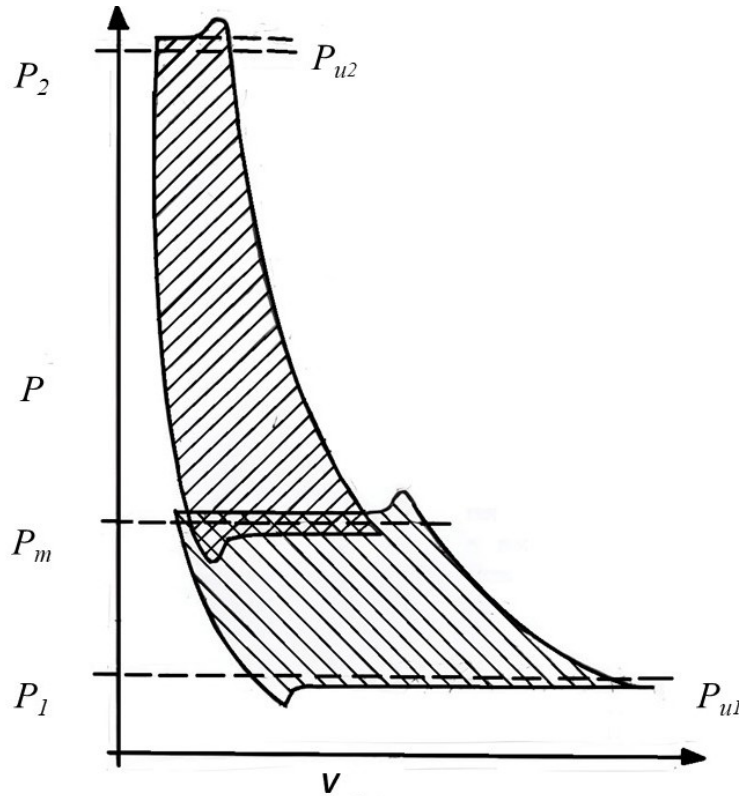


Figure 2.1: Indicator diagram of a two-stage compression screw compressor with overlapping compression phases at intermediate pressure P_m . The diagram demonstrates the relationship between pressure (P) and volume (V) across both stages, highlighting the compression process from the initial suction pressure P_{u1} to the final discharge pressure P_2 [35].

In reciprocating compressors, the stage pressure ratio determines the maximum outlet pressure and, subsequently, the outlet temperature during polytropic compression. Stages exhibiting comparable pressure ratios (P_2/P_1) typically require equivalent power consumption. In oil-injected screw compressors, the maximum discharge pressure is constrained by the pressure differential between suction and discharge, which subsequently affects the deformation of the casing and rotors. This also impacts the bearing load, especially on the outer rotor thrust bearing. Although the injected oil possesses a large heat capacity that maintains relatively low temperatures in the rotors and casing, the air temperature may stay elevated, presenting design issues with heat dissipation and pollution thresholds (δP) [35].

The design of multi-stage screw compressors encounters various obstacles, such as bending deformation of screw rotors, the longevity of rolling bearings, regulation of oil and air

temperatures, and the management of condensate formation in separator vessels, as noted by [36]. These parameters must be meticulously evaluated to guarantee optimal compressor performance, particularly in high-pressure applications.

The study by [37] examines high-pressure screw compressors as a viable alternative to other compressor designs, especially considering the global emphasis on environmental conservation and energy efficiency. The document emphasises the potential for high-pressure screw compressors in the refrigeration industry, particularly when carbon dioxide (CO_2) is favoured as a refrigerant, and in fuel gas applications where natural gas is the chosen medium. Both applications necessitate compressed fluids at pressures reaching 10 MPa. To enhance compressor efficiency in high-pressure applications, critical areas for further investigation include the optimisation of rotor profiles, identification of the optimal lubricant quantity, and regulation of lubricant viscosity.

Madhav (2003) examined the application of screw compressors in natural gas, highlighting critical parameters such built-in volume ratio, pressure ratio, rotor profile design, material selection, and the selection of bearings and seals [38]. These factors are essential for the advancement of screw compressors designed for natural gas, which is widely utilised for heating, electricity generation, and as a raw material in chemical production. The research emphasises the internal creation of a prototype with 'N' profile rotors, which shown improved performance in natural gas applications. The study emphasises the significance of adequate packaging, suitable lubricant selection, efficient filtering, and prompt maintenance to guarantee the reliability and efficiency of high-pressure screw compressors.

Hauser et al. [39] devised a chamber-based model to examine the operational attributes of an oil-free two-stage screw compressor. Their simulations of power usage and volumetric efficiency in both phases closely aligned with the experimental outcomes. The intermediate pressure is determined by the compressor's rotational speed, particularly when a constant gear ratio exists between the first and second stages. The research indicated that adjusting intermediate pressure could lead to substantial decreases in power use. Liu et al. [40] employed a mathematical model to analyse the performance of a two-stage oil-free screw compressor across diverse operating circumstances. Their findings suggested that the volumetric and indicated efficiencies of the second stage are more responsive to variations in operating conditions compared to those of the first stage.

Andres et al. [41] conducted transient simulations utilising Computational Fluid Dynamics (CFD) on a gear-driven, oil-free screw compressor. The outcomes, encompassing flow rate and power usage, aligned well with experimental data. Cipollone et al. [42] advanced this

research by formulating a detailed mathematical model for a dual-stage sliding vane rotary compressor, with pressure-swirled oil atomisers in each stage and an air-to-air intercooler situated between the stages. Their dual-stage compressor technology exhibited an energy-saving capability of up to 9.5%.

Murgia et al. [43] evaluated the efficacy of traditional single-stage sliding vane rotary compressors against two-stage compressors including interstage cooling, accomplished using either an intercooler or oil injection. Their theoretical analysis suggested that the proposed two-stage compressor with oil injection may realise energy savings of up to 10%. Experimental tests corroborated the cooling efficacy of interstage oil injection; however, these trials were confined to the second-stage compressor.

Ultimately, [44] investigated the impact of interstage oil injection in a dual motor-driven two-stage screw air compressor. The research altered the interstage oil injection flow rate and compressor rotational speed, assessing performance based on specific power, volumetric efficiency, and adiabatic efficiency. The findings indicated that proper interstage oil injection markedly enhances compressor performance, especially volumetric efficiency, but excessive oil flow in the second stage resulted in decreasing returns and heightened power usage.

These studies underscore the necessity of meticulous design, optimisation, and validation of multi-stage screw compressors for high-pressure applications. Through the optimal adjustment of rotor profiles, oil injection, and operational parameters, multi-stage compressors can achieve substantial energy savings and enhanced performance across diverse high-pressure industrial applications.

2.4 Summary

The literature study emphasises the increasing significance of high-pressure screw compressors, propelled by the global emphasis on environmental conservation and energy efficiency, especially in refrigeration and natural gas compression applications. Although high-pressure screw compressors are becoming increasingly popular, the majority of current design software is restricted to single-stage layouts, resulting in a considerable deficiency in the advancement of efficient multi-stage designs. The traditional method, which depends on multi-chamber models for manual mapping of specific stages, is both iterative and labour-intensive. This method becomes progressively intricate when considering several factors that must adhere to the conservation of mass and energy throughout all stages, hence complicating the optimisation process

and hindering the identification of the optimal parameter combination.

Moreover, whereas many studies have concentrated on improving the geometry and performance of single-stage screw compressors, there is a paucity of research concerning the design of multi-stage compressors. The cyclical characteristics of conventional modelling techniques, along with the difficulties in handling the interrelation of parameters like pressure ratio, rotor profile, and operational conditions, highlight the necessity for more sophisticated methodologies. As of now, there are no published studies that investigate the application of automated machine learning frameworks for the optimisation of multi-stage screw compressors. This framework would markedly decrease the time needed for parameter optimisation while concurrently enhancing the accuracy and efficiency of high-pressure screw compressor designs.

The research indicates that, despite significant advancements in screw compressor development, there exists a distinct possibility to enhance the industry by employing automated optimisation techniques, especially for multi-stage high-pressure applications. The implementation of these sophisticated techniques will provide more efficient and sustainable compressor designs, in accordance with global energy conservation objectives and industrial requirements.

Chapter 3

Research Aims and Contribution to Knowledge

The design and optimisation of multi-stage screw compressors pose considerable challenges due to their intrinsic complexity and the constraints of current tools and approaches. Conventional methods frequently fail to concurrently optimise essential parameters, including profile clearances, geometrical specifications, fluid injection variables, and operational conditions, especially in high-pressure applications surpassing 18 bar, as required by sectors such as oil and gas and offshore exploration. Moreover, although proficient in resolving conservation laws, traditional physics-based solutions are inadequate for multi-dimensional optimisation and necessitate computationally demanding iterative procedures. This research seeks to address these deficiencies by developing a novel optimisation and modelling framework that incorporates sophisticated soft computing methods—specifically Genetic Algorithms and Bayesian Optimization—to improve performance forecasting and facilitate parameter tuning. This work addresses these problems, enhancing the design of multi-stage screw compressors for improved efficiency, dependability, and application in high-pressure industrial environments. This research seeks to do a comparative economic analysis of single-stage versus multi-stage screw compressors, assessing lifespan costs, energy efficiency, and overall economic feasibility.

3.1 Aims of research

The primary aim of this research is to develop an advanced optimisation and modelling framework for multi-stage screw compressors. This framework integrates both conventional chamber models and cutting-edge machine learning techniques to predict compressor performance accurately, while also reducing time and computational resources. Additionally, this research seeks to validate the developed tool experimentally and perform a comprehensive economic analysis, comparing the efficiency and cost-effectiveness of single-stage and multi-stage screw compressors.

Objective 1: Performance Optimisation of Screw Compressors

- Investigate the influence of critical parameters, including profile clearances, rotor geometry, and fluid injection, on the performance of screw compressors.
- Developing a novel optimisation method employing soft computing techniques such as Bayesian, Genetic Algorithms and other evolutionary strategies to optimise screw compressor parameters, aiming to reduce time requirements and computational efforts.

Objective 2: Modelling Framework for Multi-Stage Screw Compressors

- Establish a comprehensive framework for predicting the performance of multi-stage screw compressors by integrating conventional chamber models with machine learning techniques.
- Incorporating the newly developed optimisation method into the advanced modelling tool to enable real-time performance prediction and optimisation.
- Design and construct a two-stage air screw compressor for experimental testing and validation of the advanced modelling tool.

Objective 3: Economic Analysis of Multi-Stage Screw Compressors

- Perform a comprehensive economic analysis of single-stage and multi-stage screw compressors, evaluating lifecycle costs, energy efficiency, and operational expenses for power levels ranging from 22-315 kW and delivery pressures of 6-12 bar.

3.2 Methodology

This research follows a structured approach to optimize multi-stage screw compressors by integrating advanced optimization, modeling, experimental validation, and economic analysis.

The study begins with a literature review to identify gaps in existing optimization techniques. A parametric analysis assesses the influence of key design parameters such as rotor

geometry, profile clearances, and fluid injection characteristics, providing insights for performance enhancement.

A robust customised optimization framework is developed using Genetic Algorithms and Bayesian Optimization, balancing exploration and exploitation to efficiently determine global optima. Bayesian Optimization, in particular, reduces computational cost by efficiently navigating complex design spaces.

A hybrid modeling framework integrates chamber models with machine learning techniques, including Gaussian Process Regression (GPR). This combination enhances predictive accuracy while maintaining thermodynamic consistency, enabling more reliable performance assessments.

Experimental validation is conducted using a prototype two-stage screw compressor for water-well applications. Empirical results are compared with model predictions to refine the framework and ensure practical applicability.

Finally, an economic analysis evaluates lifecycle costs, energy efficiency, and manufacturability of multi-stage compressors versus single-stage systems. The results demonstrate significant operational cost savings and long-term economic benefits.

By combining parametric analysis, optimization, machine learning, experimental testing, and economic evaluation, this methodology provides a comprehensive framework for improving multi-stage screw compressor design and efficiency.

3.3 Contribution to knowledge

This research significantly advances screw compressor technology, particularly in optimisation, modelling, experimental validation, and economic analysis of multi-stage screw compressors. This research's principal contributions are as follows:

- **Tailored Optimisation Method:** This study presents a new optimisation method utilising modern soft computing techniques, such as Genetic Algorithms and Bayesian Optimisation, specifically designed for the enhancement of screw compressor design and performance. The research highlights how resolving constraints in current optimisation approaches reveals the influence of important parameters—such as rotor geometry, fluid injection, and profile clearances—on compressor performance. The presented Bayesian

Optimisation framework facilitates effective parametric optimisation, minimising computational effort while attaining global optima. This contribution is crucial for enhancing compressor efficiency, therefore meeting the urgent demand for energy conservation in industrial applications.

- **Advanced Multi-Stage Modelling Framework:** A notable accomplishment is the creation of a hybrid modelling tool that combines conventional chamber models with machine learning methodologies, including Gaussian Process Regression (GPR). This approach improves the accuracy of performance predictions while decreasing the computational complexity of multi-stage screw compressor systems. The ability of GPR to assess uncertainty enhances its applicability in practical situations. Experimental validation using a prototype two-stage screw compressor for water-well applications confirms the reliability and precision of the modelling tool, rendering it an invaluable asset for the design and optimisation of high-pressure multi-stage systems.
- **Economic Analysis of Screw Compressors:** An extensive economic evaluation contrasts single-stage and multi-stage screw compressors, offering essential insights into lifetime expenses, energy efficiency, and economic feasibility. The research assesses multi-stage systems for power outputs ranging from 22 to 315 kW and delivery pressures between 6 and 12 bar, revealing operational cost reductions of 20 to 75% and markedly decreased lifecycle expenses. These findings provide practical recommendations for decision-makers in sectors dependent on screw compressors, emphasising the economic efficiency and sustainability of multi-stage systems.

Collectively, this research enhances the comprehension and progression of screw compressor technology by presenting a novel optimisation framework, creating a hybrid multi-stage modelling tool validated through experimental testing, and offering an economic assessment of single-stage compared to multi-stage systems. These contributions improve the efficiency, dependability, and sustainability of screw compressors, promoting ecologically responsible design and decreasing industrial energy use.

Chapter 4

Performance Optimisation of Screw Compressors

4.1 Introduction

This chapter outlines the creation of two novel optimisation frameworks aimed at tackling the intricate issues faced in screw compressor technology. These frameworks stem from comprehensive research designed to improve the efficiency, reliability, and performance of screw compressors via advanced optimisation approaches. The initial framework, known as the evolutionary framework, utilises an evolutionary methodology combined with a chamber model to assess thermodynamic performance. It is explicitly engineered to address both single-objective and multi-objective optimisation challenges, delivering resilient solutions for parameter calibration and performance improvement. The second framework, termed the Bayesian framework, integrates the conventional chamber model with machine learning methodologies to enhance predictions of thermodynamic performance. This system employs Bayesian optimisation, a sequential design methodology for the global optimisation of intricate black-box functions, adeptly addressing both single and multi-objective optimisation challenges.

4.2 Conventional optimisation methods

Numerous conventional optimisation techniques are extensively utilised in the design and performance improvement of screw compressors [20]. These methods concentrate on enhancing compressor efficiency by optimising critical parameters, including rotor shape, clearances, and fluid injection. Presented here are several established classical optimisation techniques:

- **Simplex search:** The Nelder-Mead simplex algorithm is a deterministic local search method employed to identify the maxima or minima of a specified objective function inside a multidimensional space. This method is commonly known as the box complex

method, as it solely necessitates function values for optimisation, eliminating the requirement for gradient information.

- **Steepest descent:** This first-order iterative optimisation process, commonly referred to as gradient descent, is employed to identify the local minima of a differentiable function. It is extensively utilised for seamless and ongoing optimisation challenges.
- **Newton's method:** This iterative technique is employed to identify the extrema (minima or maxima) of differentiable functions. In contrast to the steepest descent approach, Newton's method employs second-order derivative information (Hessian) to achieve accelerated convergence.
- **Davidon-Fletcher-Powell's method:** A quasi-Newton approach resolves the secant equation nearest to the present estimate while adhering to the curvature requirement. This approach necessitates both the objective function and its gradient, providing a more efficient resolution than steepest descent.
- **Random search:** A gradient-free optimisation method appropriate for functions that are discontinuous or non-differentiable. This methodology is commonly known as direct search, derivative-free, or black-box optimisation. It is utilised for investigating the design space when gradient information is either unavailable or ineffective.
- **Grid search:** Like random search, grid search identifies optimal parameters from a specified range of values. It streamlines the trial-and-error methodology, facilitating a comprehensive exploration within a defined parameter area.
- **Search along coordinate axes:** This numerical optimisation technique confines the search direction to the coordinate axes of the input space, thereby diminishing computing complexity. It is employed when the search space requires systematic exploration, one dimension at a time.
- **Powell's method:** A derivative-free optimisation technique employed to identify the local minima of real-valued functions. Powell's approach initiates with a set of search parameters orientated along the coordinate axes and subsequently updates the search directions through iterative processes.
- **Hooke-Jeeves method:** This method, sometimes referred to as pattern search, monitors the search direction as it advances from one location to another. It prevents reverting to the initial point with each new search location, facilitating a more seamless and effective investigation of the design area.

While conventional methods provide foundational techniques for optimisation, their limited global search capabilities and inefficiency in high-dimensional, multi-modal spaces have driven the adoption of more advanced approaches. Evolutionary algorithms—such as Genetic Algorithm (GA), Accelerated GA, and CMA-ES—have demonstrated strong global convergence and flexibility across complex compressor optimisation problems. Furthermore, Bayesian Optimisation offers a data-efficient, uncertainty-aware global search strategy, particularly suitable for expensive black-box evaluations. Based on comparative analysis and application suitability, Bayesian Optimisation was selected in this study for surrogate-based model optimisation, whereas evolutionary algorithms were applied in conjunction with the chamber model. Detailed implementation of both frameworks is discussed in the subsequent sections.

4.3 Evolutionary optimisation framework for screw compressors

The evolutionary framework incorporates a chamber model to assess the thermodynamic efficiency of screw compressors alongside sophisticated evolutionary algorithms for optimisation. The Genetic Algorithm (GA) is the principal optimisation technique among these algorithms, owing to its strong global search abilities and flexibility to intricate design challenges. Furthermore, many evolutionary algorithms are included into this framework to improve optimisation efficiency, offering adaptability according to particular problem needs [45]. This chapter contains a comprehensive description of these algorithms and their implementation in the following parts.

4.3.1 Genetic Algorithm

A Genetic Algorithm (GA) is a population-based optimisation technique used to find solutions to complex problems. In the context of screw compressor optimisation, a GA can be employed to adjust compressor parameters for optimal performance [46]. This study utilises the GA implementation embedded within the GT-SUITE software package developed by Gamma Technologies, which provides an integrated environment for simulation-based optimisation of thermofluid systems. The GA module in GT-SUITE supports both single and multi-objective optimisation, with configurable options for population size, generation count, crossover and mutation rates.

The basic steps of a GA are as follows:

1. **Initialization:** Create an initial population of potential solutions (chromosomes) with varying parameter values.
2. **Fitness Evaluation:** Evaluate the fitness of each chromosome using an objective function that quantifies the performance of the screw compressor.
3. **Selection:** Select the best-performing chromosomes for reproduction based on fitness values.
4. **Crossover:** Perform recombination on parent chromosomes to create new offspring.
5. **Mutation:** Introduce small random changes to maintain population diversity.
6. **Replacement:** Replace the old population with the new population of offspring.
7. **Termination:** Repeat steps until a termination condition is met.

The genetic algorithm iteratively evolves the population towards optimal solutions. The key equations are:

$$f(x) = \text{Fitness function where } x \text{ represents a chromosome} \quad (4.1)$$

$$C(x_1, x_2) = \text{Crossover operator combining two parents } x_1 \text{ and } x_2 \quad (4.2)$$

$$M(x) = \text{Mutation operator applying small changes to chromosome } x \quad (4.3)$$

As shown in Figure 4.1, the Genetic Algorithm operates by iteratively evolving the population through key steps such as crossover, mutation, and fitness evaluation.

The characteristic parameters used for GA, including population size, number of generations, mutation and crossover rates, are listed in Section 4.7 (see Table 4.5) for clarity. Additionally, the concept of seed size, which influences convergence and diversity in population-based algorithms, is discussed in Section 4.7.1.

The GA configuration in GT-SUITE was tuned based on a trade-off between search space coverage and computational efficiency. The software automatically handles constraint boundaries and supports adaptive parameter tuning in its Accelerated GA variant.

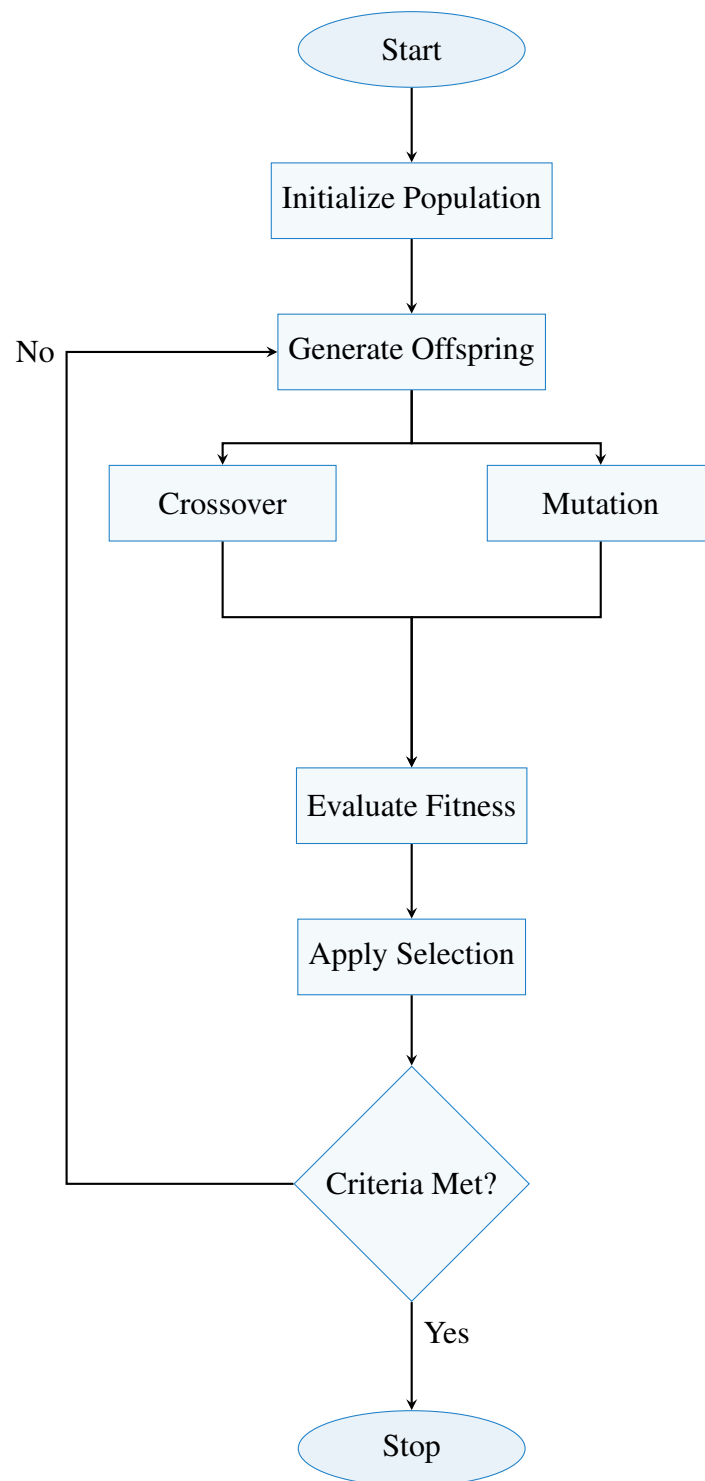


Figure 4.1: Flowchart depicting the working of a Genetic Algorithm (GA) for single-objective and multi-objective optimisation. The process begins with population initialization, followed by offspring generation, crossover, mutation, fitness evaluation, and selection. The algorithm iteratively evolves until termination criteria are met.

4.3.2 Alternative algorithms in the Evolutionary framework

Beyond the Genetic Algorithm (GA), the evolutionary framework incorporates multiple optimisation algorithms, each suited for different problem complexities and computational constraints. This section provides a mathematical overview of key alternative algorithms used in this framework [46, 47, 48].

Nelder-Mead simplex algorithm

The Nelder-Mead Simplex Algorithm is a derivative-free method for function minimisation that operates through a sequence of transformations—*reflection*, *expansion*, *contraction*, and *shrinkage*—on an n -dimensional simplex [49]. Given an objective function $f(x)$, it evaluates function values at the vertices of a simplex and updates the worst-performing vertex iteratively.

The reflection step is computed as:

$$x_r = x_c + \alpha(x_c - x_{\text{worst}}) \quad (4.4)$$

where x_c is the centroid of the best-performing vertices, and α is the reflection coefficient.

For expansion:

$$x_e = x_c + \gamma(x_r - x_c) \quad (4.5)$$

where $\gamma > 1$ is the expansion factor. This step is used when reflection improves the function significantly.

Nelder-Mead is effective for low-dimensional problems but lacks global search capability, making it less robust for high-dimensional, multimodal landscapes.

Accelerated Genetic Algorithm (AGA)

AGA enhances standard GA by dynamically adapting genetic operators to improve convergence speed. It modifies the mutation rate P_m and crossover rate P_c based on population diversity:

$$P_m = P_{m_{\min}} + (P_{m_{\max}} - P_{m_{\min}}) \left(1 - \frac{F_{\text{best}} - F_{\text{avg}}}{F_{\text{max}} - F_{\text{avg}}} \right) \quad (4.6)$$

where F_{best} , F_{max} , F_{avg} denote the best, maximum, and average fitness values, respectively [?].

This adaptive mechanism allows AGA to maintain a balance between exploration and exploitation, leading to faster convergence in large-scale design problems.

Covariance Matrix Adaptation Evolution Strategy (CMA-ES)

CMA-ES is an advanced stochastic, derivative-free optimisation method designed for non-linear and non-convex continuous problems. It updates a multivariate normal distribution's covariance matrix to guide the search [47]:

$$C_{t+1} = (1 - c)C_t + c \sum_{i=1}^{\lambda} w_i (x_i - \mu_t)(x_i - \mu_t)^T \quad (4.7)$$

where C_t is the covariance matrix at iteration t , w_i are weight coefficients, and μ_t is the population mean.

Unlike traditional GAs, CMA-ES self-adapts search directions, making it particularly effective for high-dimensional optimisation.

Brent's method

Brent's method is a univariate optimisation technique combining the bisection method, secant method, and inverse quadratic interpolation [48]. Given a function $f(x)$, it iteratively refines the interval $[a, b]$ by computing:

$$x_{\text{new}} = x_{\text{prev}} - f(x_{\text{prev}}) \frac{x_{\text{prev}} - x_{\text{prev2}}}{f(x_{\text{prev}}) - f(x_{\text{prev2}})} \quad (4.8)$$

where x_{prev} and x_{prev2} are previous iterates.

While efficient for univariate problems, it lacks scalability for high-dimensional applications.

Discrete grid method

The discrete grid method applies iterative bisection to a predefined solution space, refining the search region until convergence. Given an initial range $[x_{\min}, x_{\max}]$, it evaluates:

$$x_k = x_{\min} + k \frac{x_{\max} - x_{\min}}{N} \quad (4.9)$$

where N is the number of grid points.

Despite its simplicity, this method suffers from slow convergence in continuous-variable problems.

4.3.3 Comparison and selection of algorithms

Table 4.1 presents a comparative analysis of the discussed algorithms in terms of search capability, computational efficiency, and suitability for high-dimensional problems.

Table 4.1: Comparison of evolutionary and alternative algorithms

Algorithm	Global Search	Efficiency	Best Use Case
Genetic Algorithm (GA)	High	Moderate	Broad Applications
Nelder-Mead Simplex	Low	High	Low-dimensional search
Accelerated GA (AGA)	High	High	Large-scale problems
CMA-ES	High	Moderate	High-dimensional non-linear problems
Brent's Method	Low	Very High	Univariate optimization
Discrete Grid Method	Very Low	Low	Simple bounded problems

While Brent's method and the discrete grid method are available in the framework, they are generally not recommended for most cases, as GA, CMA-ES, and Nelder-Mead Simplex exhibit superior convergence properties.

4.3.4 Optimisation procedure

The optimisation framework integrates SCORG [9] for thermodynamic analysis and GT-SUITE [46] for evolutionary optimisation. This workflow enables both single- and multi-objective optimisation, as illustrated in Figure 4.2.

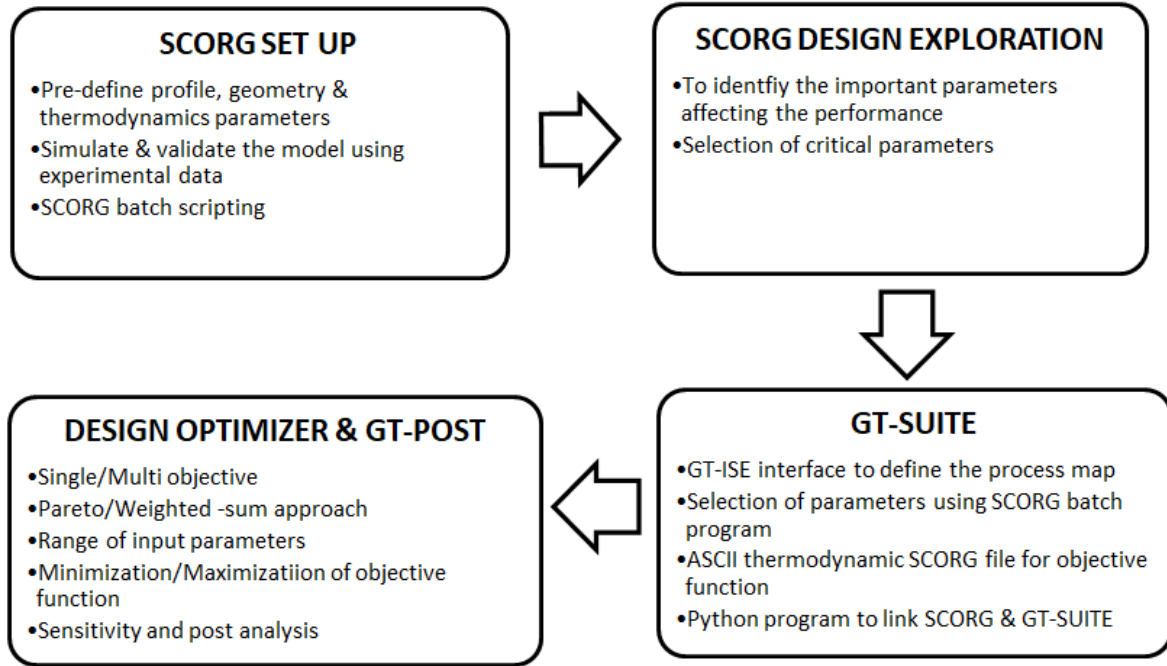


Figure 4.2: Workflow of the evolutionary optimisation framework [20]

Multi-chamber thermodynamic model

SCORG employs a multi-chamber model to predict compressor performance under varying conditions. The optimisation process involves:

1. **Input Parameter Definition:** Key design parameters such as *rotor geometry* ($L/D, \phi, VI$), *clearances* (GAPI, GAPR, GAPA), and *injection properties* ($P_{oil}, T_{oil}, D_{oil}, \theta_{oil}$) are set based on design constraints.

2. **Thermodynamic Evaluation:** The chamber model computes key performance metrics:

$$\eta_{vol} = \frac{\dot{m}_{actual}}{\dot{m}_{theoretical}}, \quad \eta_{isen} = \frac{h_{isen} - h_{suc}}{h_{dis} - h_{suc}} \quad (4.10)$$

3. **Parameter Sensitivity Analysis:** Influential parameters affecting efficiency and power consumption are identified for optimisation.
4. **Data Transfer to GT-SUITE:** The evaluated performance data is exported for *evolutionary-based optimisation*.

This integrated approach ensures an efficient methodology for optimising screw compressor designs while minimising computational cost and maximising performance improvements.

Evolutionary optimisation algorithms

GT-SUITE is a multi-disciplinary simulation and optimisation tool widely used in mechanical engineering [46]. It employs advanced evolutionary algorithms, including Genetic Algorithms (GA), Covariance Matrix Adaptation Evolution Strategy (CMA-ES), and Accelerated Genetic Algorithms, to optimise multi-variable design problems. The optimisation process involves:

1. **Process Map Development:** Thermodynamic data from SCORG is used to construct a process map, defining relationships between design variables and performance metrics.
2. **Defining Constraints and Objectives:** Using the GT-ISE interface, design constraints (P_{dis} , η_{isen} limits) and optimisation goals (minimising specific power, maximising efficiency) are set.
3. **Optimisation Execution:** The evolutionary algorithm iteratively updates design parameters, evaluates performance, and converges towards an optimal solution.
4. **Post-Processing and Sensitivity Analysis:** Optimised solutions are analysed for performance improvements, and sensitivity studies assess robustness under varying conditions.

Integrated optimisation workflow

The integration of SCORG for thermodynamic predictions and GT-SUITE for evolutionary optimisation ensures an efficient workflow:

- **High Accuracy:** The chamber model in SCORG provides precise performance predictions.
- **Computational Efficiency:** Evolutionary algorithms efficiently explore design spaces, reducing computation time.
- **Scalability:** The framework is adaptable to different compressor designs and industrial applications.

- **Comprehensive Optimisation:** Both thermodynamic and mechanical aspects are considered, enhancing efficiency and reliability.

This integration enables data-driven, systematic optimisation, improving screw compressor performance and operational efficiency.

4.4 Bayesian optimisation framework for screw compressors

The Bayesian framework developed in this study integrates a chamber model with a machine learning model to enhance the accuracy of thermodynamic performance predictions for screw compressors. This hybrid approach leverages physics-based models for fundamental calculations while utilising data-driven techniques to capture complex, non-linear interactions. The primary optimisation algorithm employed is Bayesian Optimisation (BO), which is particularly suited for computationally expensive black-box functions [50, 51].

4.4.1 Bayesian optimisation

Bayesian optimisation (BO) constructs a probabilistic model of the objective function, iteratively refining predictions as new data is acquired. Using Gaussian Processes (GP), BO estimates both the expected value and uncertainty of the objective function, enabling an adaptive search strategy that balances exploration (sampling uncertain regions) and exploitation (focusing on high-performing areas). This method is particularly effective for screw compressor design due to the high computational cost of performance evaluations [52, 53].

Key advantages of BO include:

- **Data Efficiency:** Minimises the number of function evaluations, reducing computational effort while converging towards an optimal solution.
- **Uncertainty Quantification:** Utilises GP to model uncertainty, ensuring that under-explored design regions are systematically investigated.
- **Adaptive Learning:** Adjusts the acquisition function dynamically to navigate complex and non-linear design spaces effectively.

- **Global Optimisation:** Capable of identifying global optima in constrained, multi-modal design problems [54].
- **Multi-Objective Optimisation:** Supports Pareto-based optimisation for balancing competing performance criteria, such as power consumption and efficiency.
- **Integration with Machine Learning:** Enhances predictive accuracy by incorporating Gaussian Process Regression (GPR), accelerating convergence and improving reliability [55].

By integrating BO with machine learning and chamber-based modelling, this framework provides an efficient and scalable optimisation strategy for screw compressors, ensuring data-driven improvements in design performance.

Mathematical formulation of Bayesian optimisation

Bayesian optimisation (BO) is a probabilistic model-based approach to optimising expensive black-box functions. It constructs a surrogate model, typically a Gaussian Process (GP), to approximate the objective function and guide the search for the optimal solution efficiently [56, 57].

Let $f(x)$ be the objective function, where evaluations are expensive. Instead of directly optimizing $f(x)$, BO maintains a posterior distribution $p(f | \mathcal{D})$ over the function, conditioned on observed data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, where $y_i = f(x_i) + \varepsilon$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ represents noise.

Gaussian Process Regression (GPR) as a surrogate model

A Gaussian Process (GP) is defined as a collection of random variables, where any finite subset follows a multivariate normal distribution [58, 59]:

$$f(x) \sim \mathcal{GP}(\mu(x), k(x, x')) \quad (4.11)$$

where:

- $\mu(x)$ is the mean function, typically initialized as zero.

- $k(x, x')$ is the covariance function (kernel), which encodes similarity between points. A commonly used kernel is the Matérn kernel:

$$k_v(x, x') = \frac{2^{1-v}}{\Gamma(v)} \left(\sqrt{2v} \frac{\|x - x'\|}{\ell} \right)^v K_v \left(\sqrt{2v} \frac{\|x - x'\|}{\ell} \right) \quad (4.12)$$

where ℓ is the length scale, K_v is the modified Bessel function, and v controls smoothness.

Given a set of observations $\mathcal{D}$, the posterior mean $\mu_n(x)$ and variance $\sigma_n^2(x)$ at a new query point x are given by:

$$\mu_n(x) = k(x, X)K^{-1}y \quad (4.13)$$

$$\sigma_n^2(x) = k(x, x) - k(x, X)K^{-1}k(X, x) \quad (4.14)$$

where:

- $K = k(X, X) + \sigma^2 I$ is the covariance matrix.
- $k(x, X)$ is the covariance vector between the test point and observed data.
- $y = [y_1, \dots, y_n]^T$ represents the observed function values.

Acquisition function for efficient search

The next sampling point x_{next} is selected by maximising an acquisition function $\alpha(x)$, which balances exploration and exploitation [60, 61]:

$$x_{\text{next}} = \arg \max_x \alpha(x) \quad (4.15)$$

Common acquisition functions include:

- **Expected Improvement (EI):**

$$\alpha_{\text{EI}}(x) = E[\max(f(x) - f(x^*), 0)] \quad (4.16)$$

which prioritises points likely to yield improvements over the best-observed value $f(x^*)$.

- **Probability of Improvement (PI):**

$$\alpha_{\text{PI}}(x) = \Phi\left(\frac{\mu_n(x) - f(x^*)}{\sigma_n(x)}\right) \quad (4.17)$$

where Φ is the standard normal CDF, ensuring sampling at high-probability improvement regions.

- **Upper Confidence Bound (UCB):**

$$\alpha_{\text{UCB}}(x) = \mu_n(x) + \kappa \sigma_n(x) \quad (4.18)$$

where κ is a trade-off parameter, guiding the exploration-exploitation balance.

Bayesian optimisation algorithm The BO process iterates as follows:

1. Construct the surrogate model $\mathcal{G} \mathcal{P}(\mu, k)$ using available data.
2. Select x_{next} by maximising the acquisition function $\alpha(x)$.
3. Evaluate $f(x_{\text{next}})$ and update the dataset $\mathcal{D}$.
4. Repeat until convergence.

Bayesian Optimisation efficiently identifies optimal compressor design parameters with minimal evaluations, making it well-suited for multi-stage screw compressor optimisation.

As depicted in Figure 4.3, the Bayesian optimisation process iteratively refines the surrogate model, evaluates the acquisition function, and selects the next sampling point, ensuring a balance between exploration and exploitation for efficient global optimisation.

Bayesian optimisation workflow

Bayesian Optimisation (BO) follows an iterative cycle to refine the surrogate model and converge toward the global optimum. The implementation in this study was carried out using Python's `scikit-optimize` and `scikit-learn` libraries. These offer flexible control over

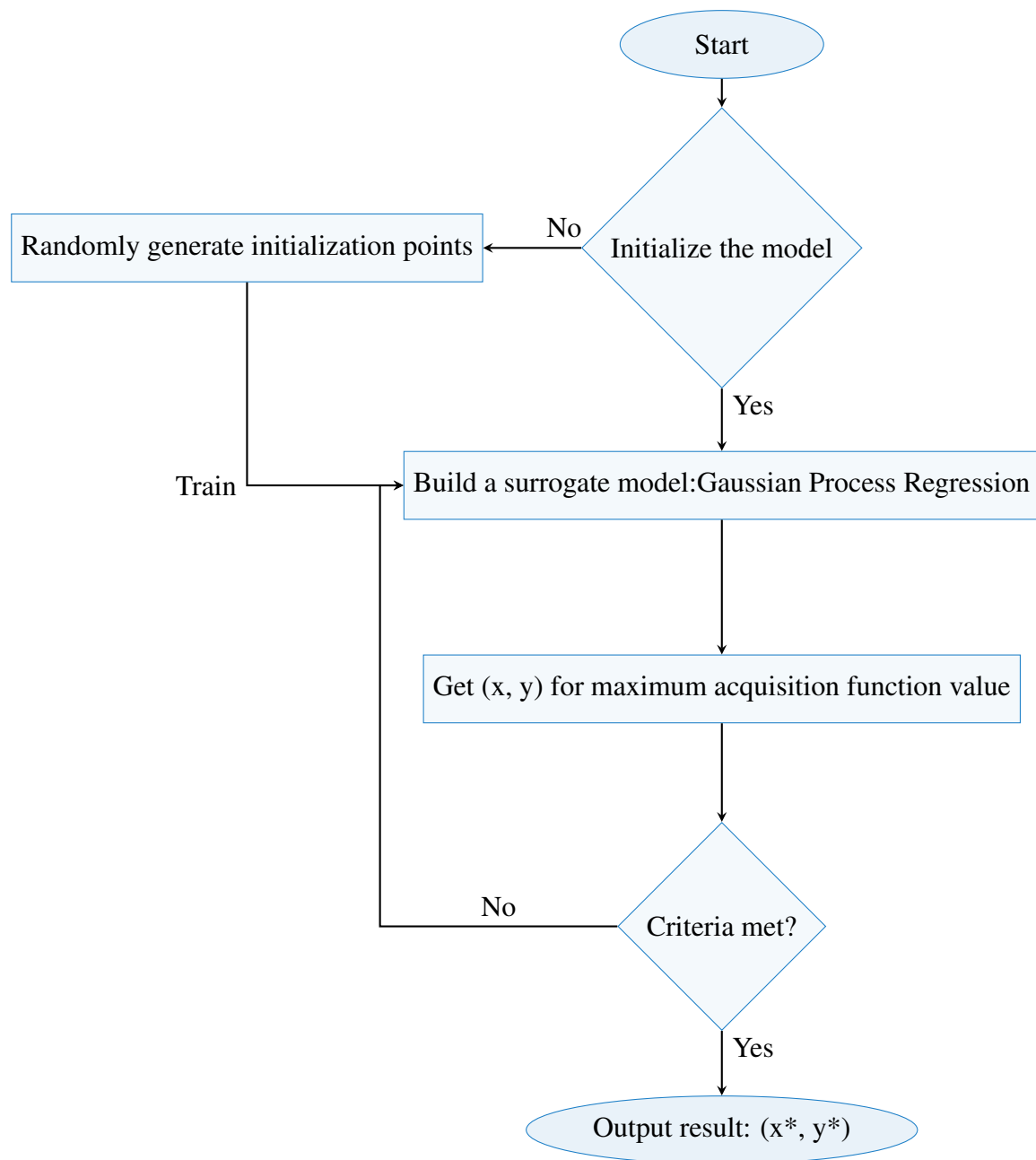


Figure 4.3: Flowchart of Bayesian Optimization showing the iterative process involving model initialization, surrogate model building, acquisition function maximization, and convergence check.

surrogate modelling, kernel selection, and acquisition function tuning, enabling robust and data-efficient optimisation.

The key steps are:

1. **Initialization:** An initial set of design points was generated using Latin Hypercube Sampling (LHS), a space-filling method that ensures diverse coverage of the design space. The objective function (based on chamber model or GPR-based surrogate) was evaluated at these points.
2. **Model Fitting:** A Gaussian Process Regression (GPR) model was used as the surrogate model to capture both the mean prediction and associated uncertainty. Multiple kernel configurations, including Radial Basis Function (RBF), Matern, and Rational Quadratic, were explored. After comparative testing, a Matern 5/2 kernel with automatic relevance determination (ARD) was selected for its superior performance in modelling non-linear trends in compressor simulations.
3. **Acquisition Function Optimisation:** The Expected Improvement (EI) acquisition function was employed to determine the next sampling point. EI was chosen after evaluating several acquisition functions such as Probability of Improvement (PI), Lower Confidence Bound (LCB), and Max-value Entropy Search (MES). EI offered a good balance between exploration and exploitation in this problem domain. The next point x_{next} was obtained by solving:

$$x_{\text{next}} = \arg \max_x \alpha(x) \quad (4.19)$$
4. **Evaluation and Update:** The chamber model (or ML surrogate, depending on the framework) was evaluated at x_{next} . The resulting value was added to the dataset, and the GPR model was retrained with the expanded dataset.
5. **Iteration:** Steps 2 to 4 were repeated until convergence criteria were met — either a threshold improvement in objective value or a maximum number of iterations (typically 40–60, depending on the application).

Extensive experimentation with kernel functions and acquisition strategies was carried out prior to final selection. This tuning process ensured that the surrogate model captured the complex behaviour of compressor performance while maintaining computational efficiency. The entire workflow was implemented using Python 3.9, with dependency on `scikit-learn` v1.2.2, `scikit-optimize` v0.9.0, and `numpy` for matrix operations and numerical routines.

4.4.2 Alternative algorithms in the Bayesian framework

The Bayesian framework integrates various optimisation algorithms to complement Bayesian Optimisation (BO), offering flexibility for different problem structures [50, 62]. These alternative algorithms provide different search strategies depending on function smoothness, dimensionality, and computational complexity.

Nelder-Mead Algorithm

The Nelder-Mead algorithm is a derivative-free local search method that operates using a simplex—a set of $n + 1$ points in an n -dimensional space. The algorithm iteratively refines the simplex by performing reflection, expansion, contraction, and shrinkage operations.

Mathematically, the new candidate point x_{new} is determined by:

$$x_{\text{new}} = x_{\text{centroid}} + \alpha(x_{\text{worst}} - x_{\text{centroid}}) \quad (4.20)$$

where:

- x_{centroid} is the centroid of the best n points.
- x_{worst} is the worst-performing vertex in the simplex.
- α is the reflection coefficient.

This algorithm is effective for low-dimensional problems and is widely used in engineering optimisation [63].

Powell's method

Powell's method is a derivative-free optimisation technique that employs a set of conjugate search directions to minimise a function iteratively. At each iteration, the function is minimised along each direction d_k , updating the solution:

$$x_{k+1} = x_k + \alpha_k d_k \quad (4.21)$$

where:

- α_k is the step length along the direction d_k .
- d_k is a conjugate search direction, updated to maintain efficiency.

Powell's method is particularly useful when derivatives are unavailable but is limited in high-dimensional problems due to its sequential search nature [64].

Conjugate Gradient (CG) method

The Conjugate Gradient method is a powerful gradient-based optimisation algorithm designed for large-scale problems. It improves on steepest descent by selecting conjugate directions to accelerate convergence. The update rule is:

$$x_{k+1} = x_k + \alpha_k p_k \quad (4.22)$$

where:

- $p_k = -\nabla f(x_k) + \beta_k p_{k-1}$ is the conjugate search direction.
- β_k is computed using the Fletcher-Reeves or Polak-Ribière formula.

The Conjugate Gradient method is particularly effective for large-scale quadratic optimisation problems [65].

COBYLA (Constrained Optimisation BY Linear Approximations)

COBYLA is a derivative-free optimisation method designed to handle nonlinear constraints. It constructs linear approximations of constraints and optimises within feasible regions:

$$\min f(x) \quad \text{subject to} \quad g_i(x) \leq 0, \quad i = 1, 2, \dots, m \quad (4.23)$$

where $g_i(x)$ represents the inequality constraints. COBYLA iteratively adjusts the simplex while ensuring constraint satisfaction, making it useful for constrained engineering problems [66].

Particle Swarm Optimisation (PSO)

Particle Swarm Optimisation (PSO) is a population-based stochastic algorithm inspired by swarm intelligence. Each particle in the swarm moves within the search space according to:

$$v_i^{(t+1)} = wv_i^{(t)} + c_1r_1(p_i^* - x_i^{(t)}) + c_2r_2(p_g^* - x_i^{(t)}) \quad (4.24)$$

$$x_i^{(t+1)} = x_i^{(t)} + v_i^{(t+1)} \quad (4.25)$$

where:

- $v_i^{(t)}$ is the velocity of particle i at iteration t .
- $x_i^{(t)}$ is the position of the particle.
- p_i^* is the best position found by particle i .
- p_g^* is the global best position found by any particle.
- w is the inertia weight, controlling exploration vs. exploitation.
- c_1, c_2 are acceleration coefficients.
- r_1, r_2 are random numbers between 0 and 1.

PSO is highly effective for solving non-convex, high-dimensional problems and has been widely applied in engineering optimisation [67].

4.4.3 Summary of alternative algorithms

Each of these algorithms offers distinct advantages depending on the problem type:

- **Nelder-Mead:** Best for small, smooth, derivative-free problems.
- **Powell's Method:** Suitable for low-dimensional problems with few variables.
- **Conjugate Gradient:** Efficient for large-scale quadratic optimisation.
- **COBYLA:** Effective for constrained problems without derivatives.
- **PSO:** Stochastic approach ideal for high-dimensional and complex landscapes.

This flexibility allows Bayesian frameworks to adapt to diverse optimisation challenges.

4.4.4 Optimisation procedure

1. Run the Physics Solver (Chamber Model/ Machine Learning):
 - Execute the solver using a batch file.
 - Input initial parameters (suction pressure, discharge pressure, temperature, rotor speed).
2. Optimisation Setup:
 - Choose parameters to optimize (profile, geometry, or fluid).
 - Modify corresponding batch files accordingly.
3. Parameter Bounds and Initial Values:
 - Define lower and upper bounds for each parameter.
 - Specify initial values for optimisation.
4. Optimisation Method:
 - Select an optimisation method (e.g., Bayesian, Nelder-Mead, PSO, Powell, etc.).
5. Optimisation and Data Collection:
 - Start a timer to measure optimisation time.
 - Perform the optimisation.
 - Collect evaluations and objective values.
 - Display the optimisation result, total evaluations, optimal parameters, and time taken.

4.5 Multi-objective optimisation strategies for screw compressors

Design optimiser interface allows two different design approaches for multi-objective optimisation, which are as follows [20]:

- Pareto-design: This approach is used to maximize, minimize or target an output response and study its competing objectives. It gives many optimal designs considered equally optimal and not a single best design.
- Weighted-sum approach: This approach combines the multiple objectives into a single-objective function by assigning a weight function to each output. An example of how this work is shown below:

Let,

P_1 = First objective function which is to be maximized

P_2 = Second objective function which is to be minimized

The combined single-objective function as per weighted-sum approach is given as:

$$F = \frac{P_1}{P_{norm1}} - \frac{P_2}{P_{norm2}} \quad (4.26)$$

where, P_{norm1} and P_{norm2} are the normalized value for each output function so that each output function is of the same order of magnitude when combined into a single-objective function. If the values are not normalized, the single-objective function will be dominated by the output function with a larger magnitude of weight function.

This chapter has introduced two distinct optimisation frameworks tailored to address the complexities of screw compressor design, providing a robust foundation for subsequent chapters.

4.6 Parametric analysis and fluid injection effects in screw compressors

The design and performance of screw compressors are governed by a range of geometric and operational parameters that influence efficiency, reliability, and energy consumption. Establishing an appropriate range for optimization is crucial, as an excessively large or loosely defined

design space may lead to non-converging solutions that are impractical from both a performance and manufacturing standpoint. Therefore, this section investigates the impact of key parameters and fluid injection on compressor performance to identify optimal ranges that balance energy efficiency, operational feasibility, and manufacturability [68].

The study is conducted through a structured parametric influence analysis comprising the following phases:

1. **Experimental Validation:** Performance testing was carried out on a prototype two-stage screw compressor under controlled conditions to evaluate the effects of different parameters on key performance metrics.
2. **Digital Model-Based Analysis:** A simulation framework employing a chamber-model-based approach was developed to assess parameter trends and their influence on performance characteristics.
3. **Optimization Feasibility Assessment:** Insights from the experimental and numerical studies help define appropriate parameter bounds for optimization, particularly for rotor geometry, profile clearances, and fluid injection characteristics, ensuring convergence to feasible and efficient solutions.

Fluid injection plays a significant role in thermal management, sealing, and overall performance. To gain a comprehensive understanding, this study also compares the effects of oil and water injection, assessing their impact on specific power consumption, volumetric efficiency, and discharge temperature.

By integrating experimental data, numerical simulations, and optimization insights, this section provides a systematic foundation for defining constraints and input variables for the optimization framework presented in later chapters. The findings serve as a basis for enhancing screw compressor design by ensuring that optimization is conducted within a well-defined and practically viable parameter space.

4.6.1 Core parameters and their significance

In screw compressor design, several core parameters play critical roles in influencing performance, efficiency, and reliability. The primary parameters can be classified into four major

categories: input parameters (operating conditions), profile clearances, geometrical parameters, and fluid injection parameters. A holistic optimization of these interrelated parameters is essential to achieve optimal performance and minimize energy losses.

- **Input parameters:** The initial conditions, such as suction pressure (P_{suc}) and temperature (T_{suc}), influence the state of the working fluid entering the compressor and dictate the achievable compression ratio. Similarly, the discharge pressure (P_{dis}) defines the compressor's output requirements. These conditions are essential to understanding and setting the baseline for operational metrics.
- **Profile clearances:** Profile clearances, such as interlobe clearance (GAPI), radial clearance (GAPR), and axial clearance (GAPA), directly impact the compressor's sealing and leakage rates. The interlobe clearance governs the sealing between the male and female rotors, while radial and axial clearances prevent rotor-casing contact and accommodate thermal expansion, enhancing the compressor's mechanical robustness.
- **Geometrical parameters:** Geometric parameters such as the relative rotor length (L/D), wrap angle (ϕ), and built-in volume ratio (VI) influence the compressor's efficiency, pressure ratio, and capacity. The *built-in volume ratio (VI)*, defined as:

$$VI = \frac{V_s}{V_d} \quad (4.27)$$

where V_s and V_d are the suction and discharge volumes, respectively, is crucial in defining the compressor's pressure ratio. An optimized VI minimizes specific power consumption and enhances volumetric efficiency, contributing to improved thermodynamic performance.

- **Fluid injection parameters:** Fluid injection properties, including injection pressure (P_{oil}), temperature (T_{oil}), injection diameter (D_{oil}) and angle (θ), are vital for thermal management, sealing, and lubrication.

4.6.2 Performance metrics

The performance of a screw compressor is assessed using key metrics that offer insights into its energy efficiency, capacity, and thermodynamic behavior. These metrics, detailed in Appendix B, are governed by specific equations that enable precise evaluation, control, and optimisation.

By quantifying these parameters, they provide a deeper understanding of the physical processes within the compressor, facilitating improved performance and operational efficiency [20].

4.6.3 Fluid injection: oil or, water

The choice of fluid injection, and the associated injection parameters, is a key determinant of a screw compressor's thermal management, sealing, and efficiency. This study considers two different fluids—traditional oil and water—as outlined below:

Oil injection:

In conventional screw compressors, oil (ISO VG68 Grade) is commonly used as the working fluid for its superior sealing, lubrication, and cooling properties. Oil's specific heat capacity ranges from 1.65 to 2.25 kJ/kg-K, allowing effective heat absorption and transfer during the compression cycle. Oil injection provides thermal stability and lubricates moving components, reducing wear and extending operational lifespan [4].

Water injection:

As an alternative to oil, this study investigates the potential of water as the working fluid. Water has a high specific heat capacity of 4.186 kJ/kg-K, offering enhanced cooling with minimal volume compared to oil. Its lower viscosity reduces viscous drag, potentially lowering frictional losses within the compressor. Water injection, however, presents unique challenges such as poor lubrication, increased corrosion risk, and potential bacterial contamination [3]. Despite these challenges, water-injected compressors exhibit promising thermodynamic advantages, operating below the dew point without oil dilution risks.

This study conducted experimental tests on an industrial screw compressor developed by Kirloskar Pneumatic Company Limited (KPCL), Pune, India, to evaluate the performance impacts of water injection. The experimental setup, results, and analysis of fluid injection effects are detailed in the following sections, with a focus on comparing the thermodynamic performance of oil and water-injected systems.

4.6.4 Experimental setup

This section details the development and configuration of a water-injected prototype based on the KAS-200 screw compressor block (airend), manufactured and assembled at KPCL. The KAS-200 is a robust, industrial-grade, oil-flooded air screw compressor designed for power ratings of 15–22 kW, operating at various pressure ratios (7.5, 8.5, 10, and 13). It features the "N" rotor profile, with a 4/5 lobe combination, a L/D of 1.55, a VI of 4.6, and a ϕ of approximately 306° . The compressor operates with a tip speed between 20–35 m/s, delivering a volume flow rate of $1.76\text{--}3.57\text{ m}^3/\text{min}$. This belt-driven compressor is powered by an electric motor, with the prototype modified to use water injection in place of oil injection. Figure 4.4 shows a cross-sectional view of the KAS-200 compressor block.

- Rotor Length-to-Diameter Ratio (L/D) = 1.55
- Male Rotor Wrap Angle (ϕ) = 306.647°
- Built-in Volume Ratio (VI) = 4.6
- Working Fluid: Air
- Maximum Chamber Volume = $175,259\text{ mm}^3$

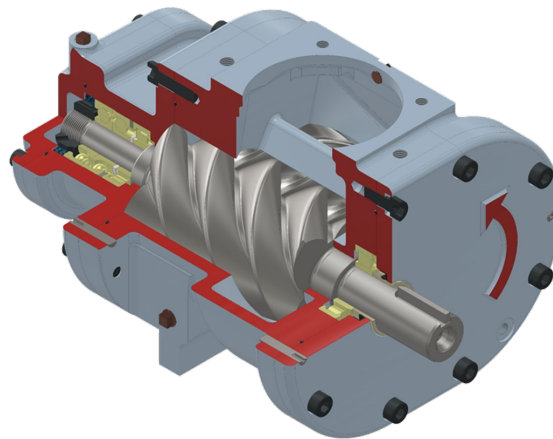


Figure 4.4: Cross-sectional view of the KAS-200 screw compressor block, featuring a male rotor with four lobes and a female rotor with five lobes, with the male rotor serving as the driving component.

To accommodate the water injection configuration, a customized test package was developed for the KAS-200 compressor. Stainless steel was selected for the air-water separator (AWS) tank and piping to prevent corrosion, and a demister pad was included to effectively remove entrained water droplets from the gas stream. Positioned just below the top vapour outlet of the separator tank, the demister pad works alongside centrifugal and gravitational separation, maintaining consistency with traditional air-oil separator principles.

The main compressor components remained unchanged from the oil-flooded configuration, with cast iron housings, medium carbon steel rotors, and anti-friction bearings for smooth operation. This consistency enables direct comparison between the oil and water-injected configurations. The system's operation is outlined in the piping and instrumentation diagram shown in Figure 4.5.

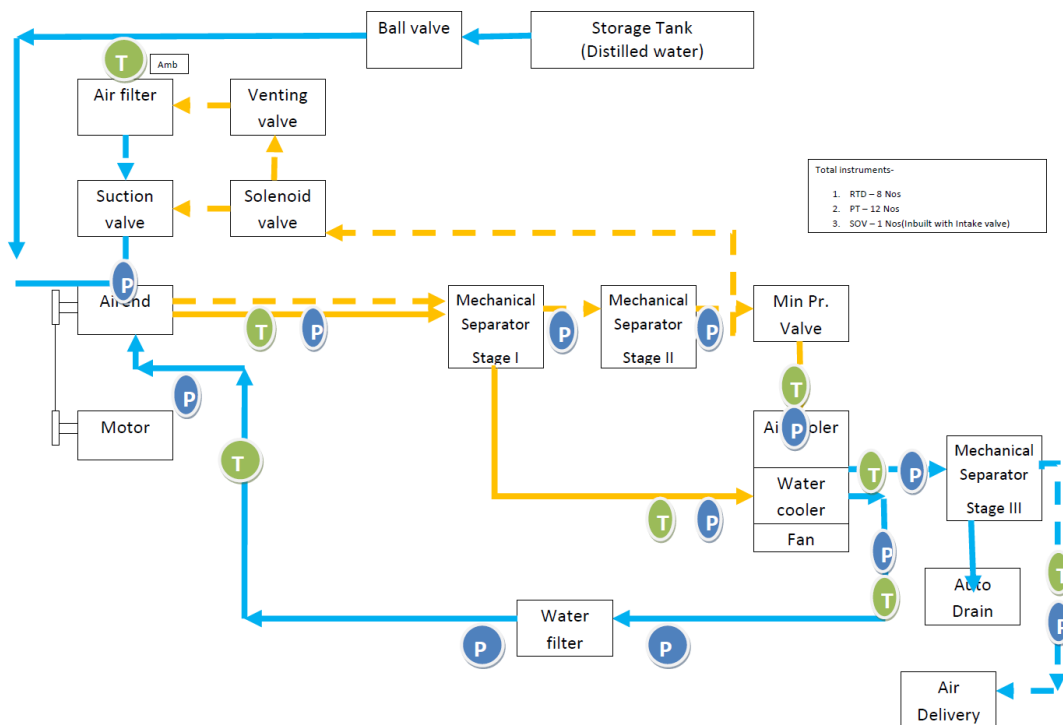


Figure 4.5: Piping and instrumentation diagram of the water-injected screw compressor test setup, illustrating flow paths and major components, including 8 Resistance Temperature Detectors (RTDs), 12 Pressure Transducers (PTs), and 1 Solenoid Valve (SOV) integrated with the intake valve.

The system operates as a closed-loop cycle: compressed air mixed with water exits the compressor block and enters the primary and secondary mechanical separators, where water is separated from the air. The separated air passes through an air cooler and a minimum pressure valve to prevent backflow before reaching a final mechanical separator, which removes the remaining moisture. Meanwhile, separated water travels through a water cooler and filter before

being reintroduced into the compressor block. Approximately 23 litres of distilled water were used in this system, distributed as follows: 17 litres in the AWS tank, and 3 litres each in the airend and cooler sections.

Figure 4.6 shows the complete water-injected screw compressor setup, providing a comprehensive view of the experimental assembly.

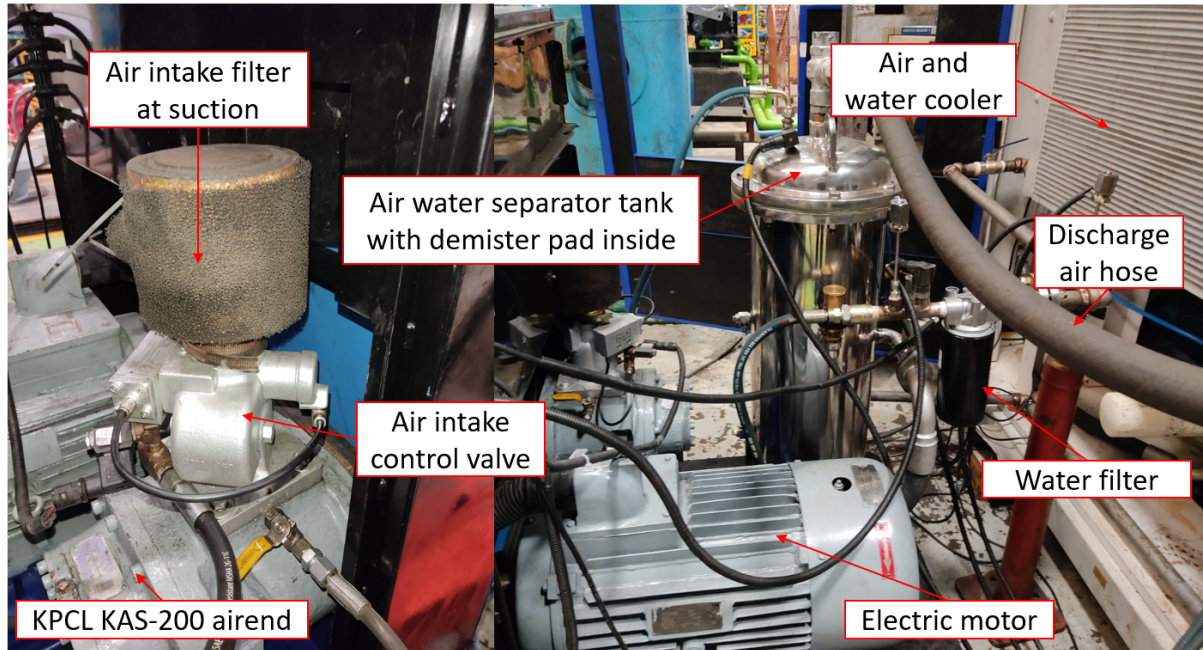


Figure 4.6: Schematic labelled diagram of the compressor test rig. The diagram illustrates the complete test rig components, including the bare KAS-200 compressor, providing a comprehensive view of the experimental setup.

4.6.5 Testing procedure

The experimental setup was designed following ISO 1217 standards for displacement compressors and ISO 5389 standards for performance assessment, ensuring accurate and reliable results. The prototype was tested using both oil and water as the injection fluid, with performance evaluated under steady-state conditions at specified operating points. Testing commenced only after thermal and mechanical equilibrium was achieved, ensuring stable parameters across pressures, temperatures, and rotor speeds.

Each test was conducted for a minimum of 10 minutes, with data collected at regular intervals and averaged to mitigate transient fluctuations. The recorded data were normalized to the specified pressure ratios and rotor speeds, providing standardized results for reliable

comparison. This meticulous approach ensured that all tests adhered to industry standards, yielding dependable performance metrics for subsequent analysis.

4.6.6 Results and discussion

This section presents the experimental results obtained from testing the KAS-200 compressor block with two different fluid injections: oil and water. The collected data facilitated the development of a digital model of the KAS-200 compressor in SCORG (Screw Compressor Rotor Grid Generation) software, as detailed in [9]. SCORG employs a chamber model approach for performance analysis [20], enabling a detailed investigation of how various parameters—such as profile clearances, geometrical factors, and fluid injection conditions—affect screw compressor performance.

4.6.7 Experimental testing results

The performance of the KAS-200 screw compressor block was evaluated under various operating conditions using both water and oil as injection fluids at a pressure ratio of 8.5. Key performance parameters measured during testing are summarized in Table 4.2.

Table 4.2: Testing Results for KAS-200 Compressor Block

P_{dis} (bar a)	W_{tip} (m/s)	P (kW)	SPC (kW/m ³ /min)	Q (m ³ /min)
Fluid Injection: Water				
8.00	32	23.56	7.032	3.35
Fluid Injection: Oil				
8.00	32	24.74	7.385	3.35

Results indicate that the water-injected configuration of the KAS-200 compressor achieved a notable improvement in efficiency compared to the oil-injected setup. Specifically, the water-injected compressor demonstrated a 4.59% reduction in SPC, reflecting enhanced operational efficiency. This improvement is primarily attributed to water's superior thermal capacity, which promotes near-isothermal compression, thus reducing energy losses.

However, the introduction of water in a compressor traditionally designed for oil flooding resulted in notable challenges. After approximately 25 hours of operation, signs of corrosion,

bacterial pollution and scaling were observed on the compressor components, as shown in Figure 4.7. These issues underscore the complexities involved in developing a reliable water-flooded screw compressor and highlight the necessity for further research and development to address these challenges effectively.

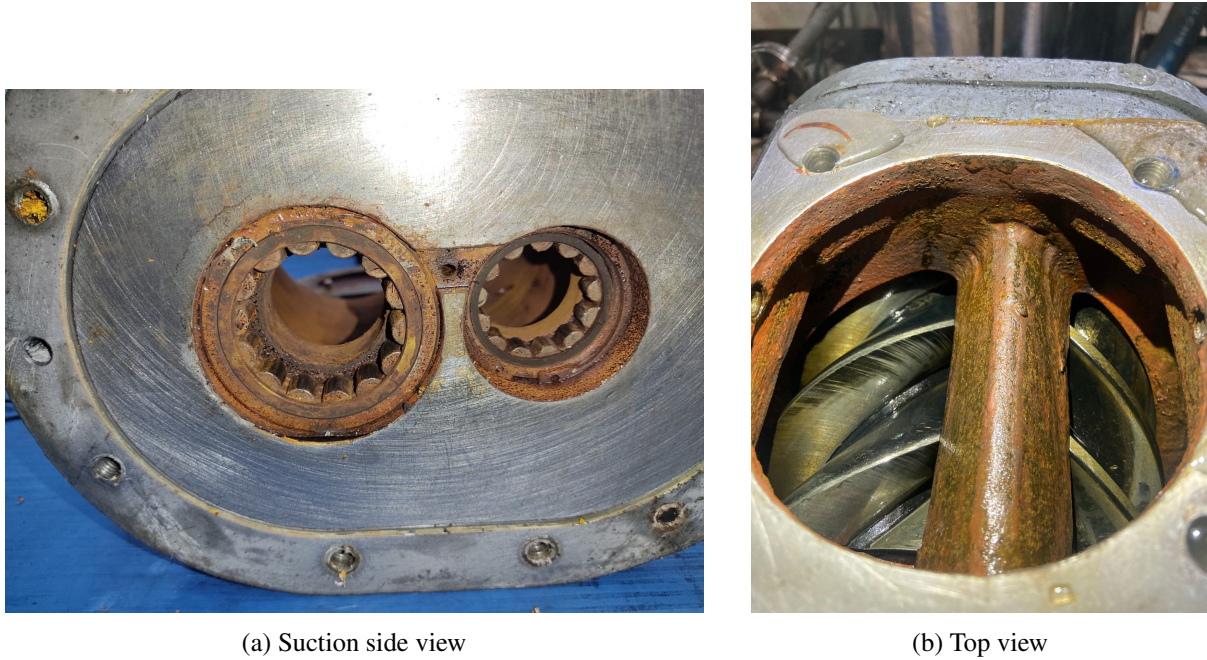


Figure 4.7: Condition of the compressor block after 25 hours of operation

4.6.8 Simulation results from chamber model analysis

The SCORG model of the KAS-200 screw compressor, calibrated with experimental data (see Section 4.6.7), was employed to conduct a parametric analysis. This analysis evaluates the effects of profile clearances, geometric characteristics, and fluid injection parameters on compressor performance.

Operating conditions:

The compressor's performance is strongly influenced by key operational parameters, including suction and discharge pressures and the rotor's tip speed. Suction and discharge pressures define the pressure ratio across the compressor, impacting power consumption and discharge temperature. An optimal pressure ratio, here set at 8.5, is critical to achieving efficient compression across typical industrial applications, where such ratios are widely required.

The next important factor is the tip speed of the male rotor, which affects both the flow rate and power consumption. Higher rotor speeds enhance flow but increase frictional losses and heat, leading to elevated SPC and potential wear. Thus, finding an optimal rotor speed is essential for maximizing efficiency and reliability. The ideal tip speed generally lies in the range of 20 to 35 m/s. The tip speed is given by:

$$W_{\text{tip}}(\text{m/s}) = \frac{\pi \times D_{\text{male}}(\text{mm}) \times N(\text{rpm})}{1000 \times 60} \quad (4.28)$$

The effects of varying suction and discharge pressures on SPC are illustrated in Figures 4.8a and 4.8b. Additionally, Figure 4.8c shows the influence of rotor tip speed on power consumption, flow rate, and SPC at a pressure ratio of 8.5.

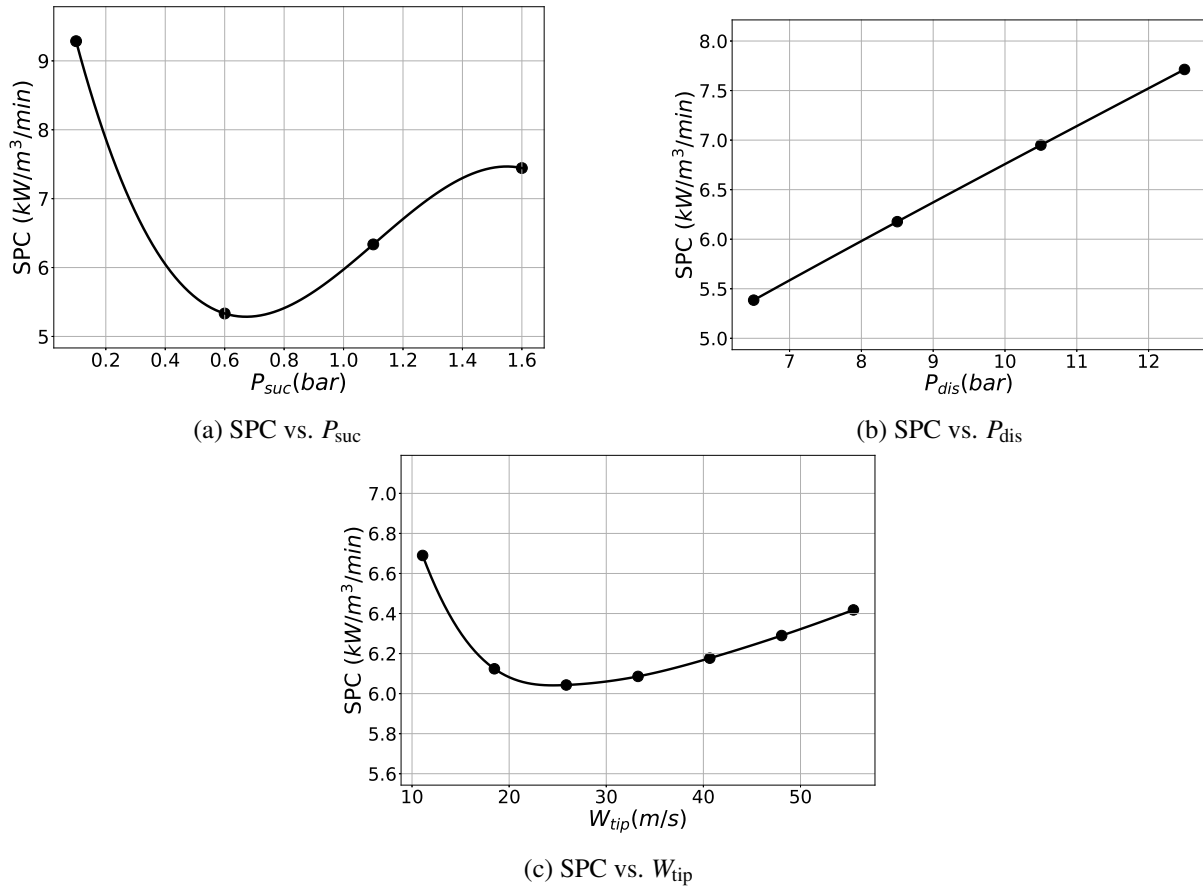


Figure 4.8: Impact of operating conditions on compressor performance: (a) and (b) illustrate the effect of suction and discharge pressures on specific power consumption, while (c) shows the influence of tip speed on screw compressor performance at a pressure ratio of 8.5.

The analysis reveals that increasing tip speed enhances flow rate and power consumption,

but at the cost of higher specific power consumption. These results underscore the importance of optimizing rotor speed to achieve an optimal balance between energy efficiency and performance.

Impact of water and oil injection on screw compressor performance:

To assess and validate the experimental trends observed with water injection relative to oil, SCORG simulations were performed. These simulations enabled a detailed comparison of the performance impacts of water versus oil as the injection fluid, as depicted in Figure 4.9. The shaded region indicates the range of variation between the two fluids, highlighting distinct performance differences. Key findings from the simulation analysis include:

- **Specific power consumption (SPC):** The water-injected screw compressor demonstrated lower specific power consumption compared to the oil-injected configuration (Figure 4.9a). This reduction in SPC suggests that water injection offers improved energy efficiency, likely due to water's higher heat capacity, which aids in more effective heat absorption and transfer during the compression process.
- **Discharge temperature (T_{dis}):** The water-injected compressor also exhibited significantly lower discharge temperatures, generally within a range of 40 °C to 60 °C (Figure 4.9b). This cooler discharge temperature is beneficial for applications sensitive to thermal effects, as it indicates that water injection supports near-isothermal compression, reducing thermal stresses and potentially extending component lifespan.

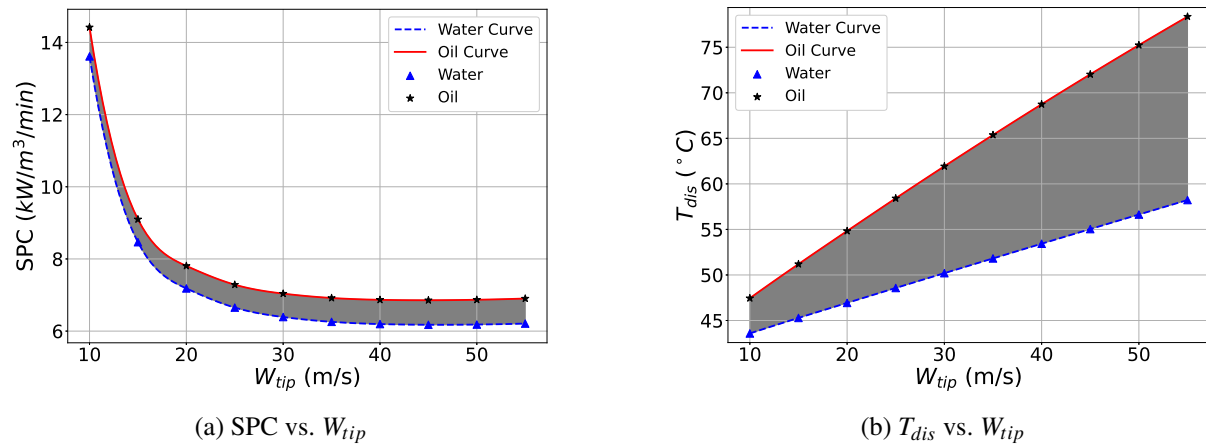


Figure 4.9: Comparison of water and oil injection effects on screw compressor performance: (a) Specific power consumption and (b) discharge temperature.

Effect of profile clearances on compressor performance:

Figure 4.10 shows the impact of profile clearances on screw compressor performance at a pressure ratio of 8.5. As profile clearances increase, performance declines due to the following factors:

- **Increased gas leakage:** Larger clearances allow more gas to escape between rotor lobes and the compressor housing, decreasing the volume of gas compressed and thereby lowering volumetric efficiency.
- **Enhanced turbulence and friction:** Larger clearances increase turbulence and friction in the gas flow, reducing adiabatic efficiency and overall compressor effectiveness.

While minimizing clearances can reduce these inefficiencies, extremely low clearances lead to exponential performance losses due to increased oil drag and potential wear on components, which can compromise compressor reliability and lifespan.

These findings highlight the importance of optimizing profile clearances to achieve balanced performance, efficiency, and durability in screw compressors.

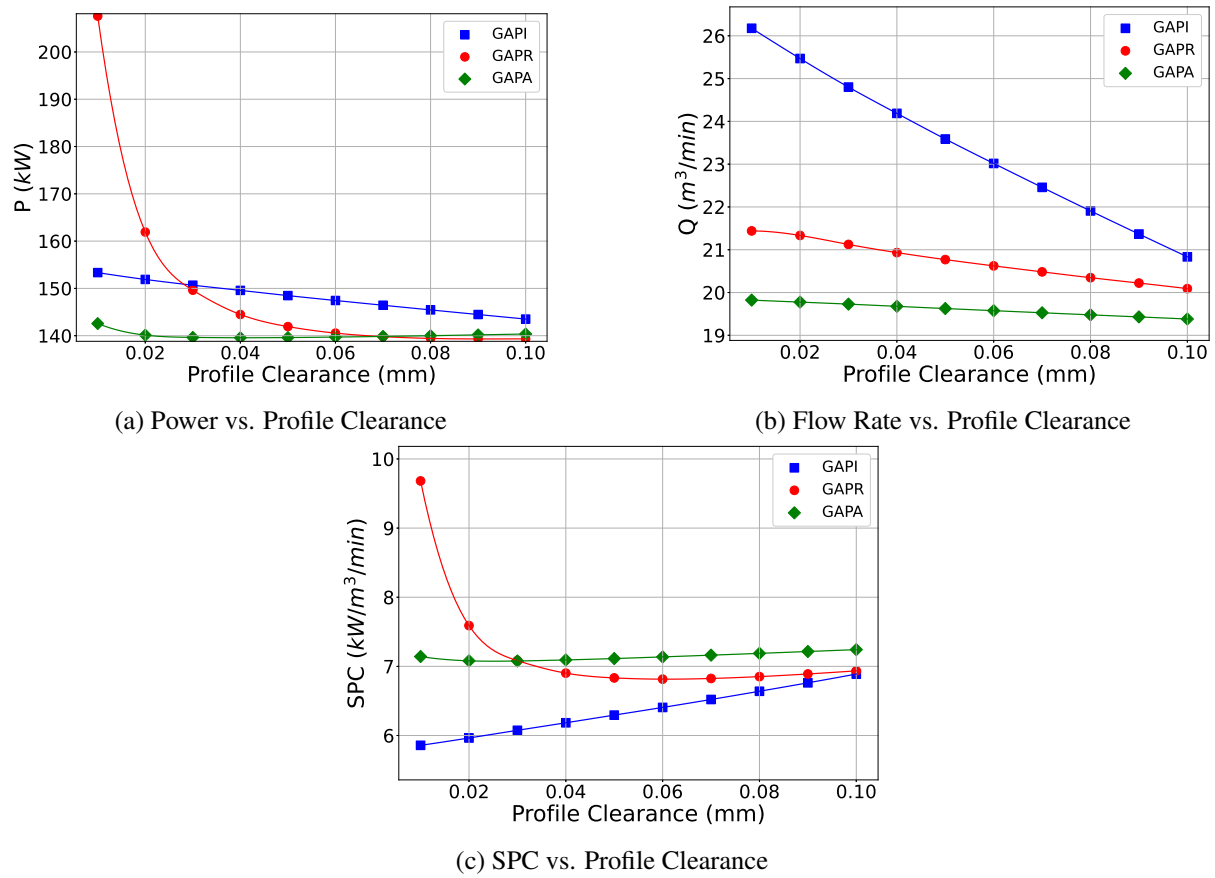


Figure 4.10: Impact of interlobe, radial, and axial clearances on screw compressor performance at a pressure ratio of 8.5.

Effect of geometrical parameters on compressor performance

Relative rotor length:

The relative rotor length, defined as the ratio of rotor length to diameter, indicates rotor slenderness. A higher L/D ratio extends the compression chamber, enabling higher pressure ratios. However, it also increases friction and heat generation, leading to elevated power consumption and potential reductions in compressor lifespan.

The impact of increasing L/D is twofold: while it enhances total displacement volume and contributes to performance gains, it also demands more power due to the added rotor mass. This increase is limited by the fixed power rating of the motor. Additionally, higher L/D ratios result in greater rotor deflection, which can affect compressor reliability. As a guideline, it is recommended to keep maximum rotor deflection within one-third of the radial clearance:

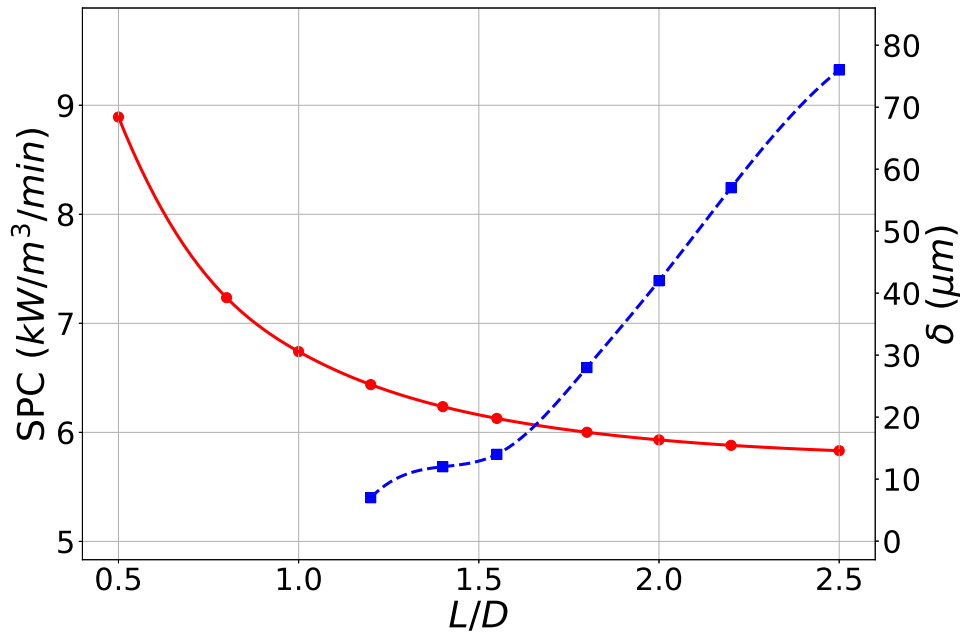


Figure 4.11: Influence of relative rotor length on specific power consumption and female rotor deflection at a pressure ratio of 8.5.

$$\text{Maximum female rotor deflection } (\delta) = \frac{1}{3} \text{ GAPR} \quad (4.29)$$

For optimal performance, L/D ratios in screw compressors generally range between 1.5 and 1.9, balancing pressure ratio, efficiency, and longevity.

As shown in Figure 4.11, increasing L/D improves SPC but also raises female rotor deflection. In the KAS-200 compressor block, an L/D of 1.55 provides a good balance, yielding high performance with minimal deflection.

Wrap angle:

The wrap angle of the male rotor defines the angular span of the rotor profile, indicating the degree of engagement between the male and female rotors. A higher wrap angle increases the compression volume, resulting in a higher discharge flow rate (see Figure 4.13). However, this also raises leakage and friction losses, leading to increased power consumption and reduced efficiency.

While a wrap angle below 300° can reduce specific power consumption by minimizing

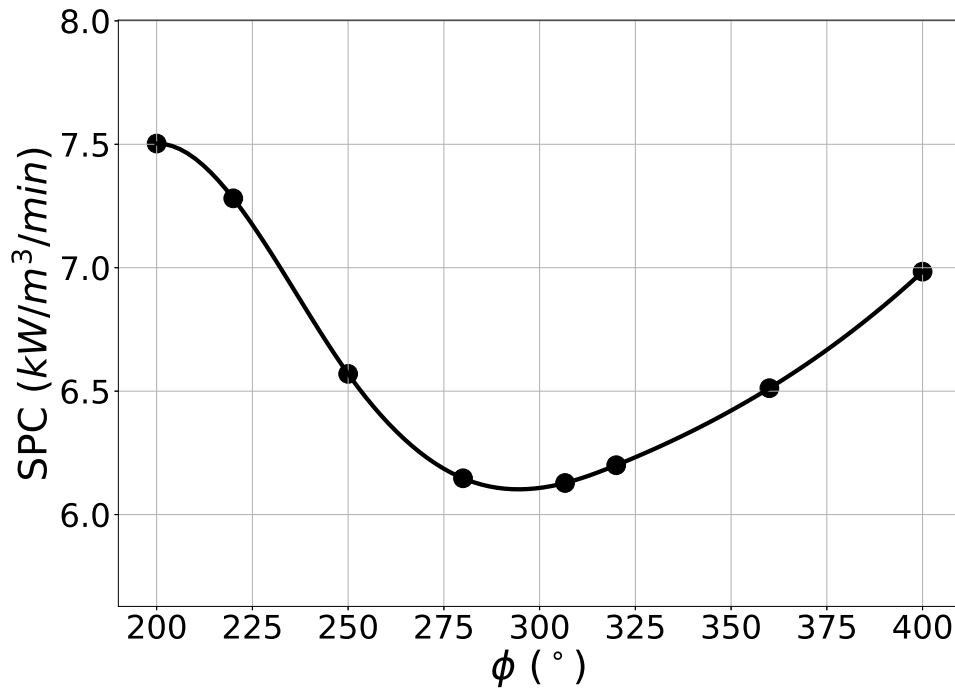


Figure 4.12: Influence of wrap angle on screw compressor performance at a pressure ratio of 8.5.

friction and chamber volume, it also expands leakage paths, adversely affecting performance, especially under high-pressure conditions. In practical applications, an optimal wrap angle typically ranges from 300° to 330° , balancing flow rate, efficiency, and durability in demanding environments.

The existing wrap angle of the male rotor in the KAS-200 compressor is 306.647° . Figure 4.13 shows the variation in specific power consumption as a function of the wrap angle. The results indicate that specific power decreases as the wrap angle is reduced. Within the tested range of 350° to 200° , the specific power varies by $0.348 \text{ kW/m}^3/\text{min}$. However, reducing the wrap angle also increases leakage areas, which can negatively affect performance.

Other rotor characteristics, such as actual chamber volume and displacement volume, increase as the wrap angle decreases, counteracting the effects of increased leakage through blow holes and sealing line length (see Figure 4.14). While these changes can enhance performance under certain conditions, higher leakage rates could reduce efficiency, especially under high-pressure ratios or extreme working conditions. Deflection analysis of the rotors showed that changes in the wrap angle had an insignificant impact on deflection. The effective performance gain from reducing the wrap angle to 260° (beyond which further gains are minimal) is approximately 1.9%.

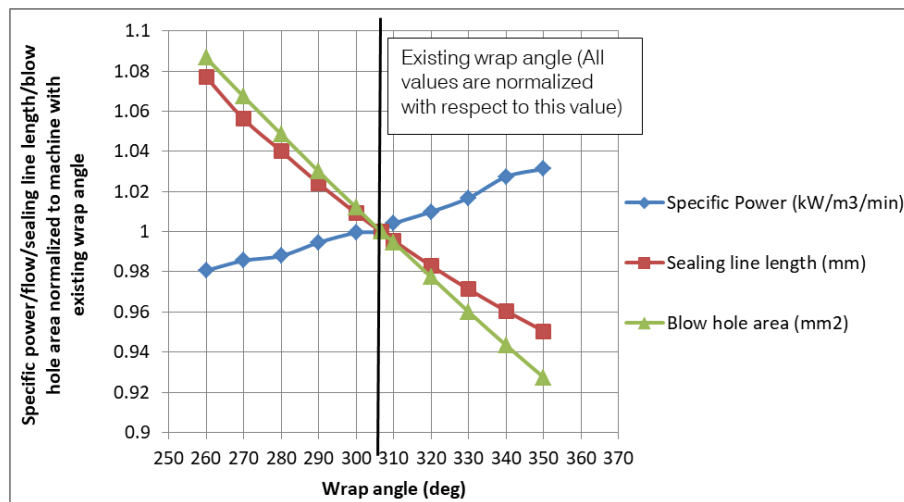


Figure 4.13: Variation in specific power and leakage areas with respect to wrap angle.

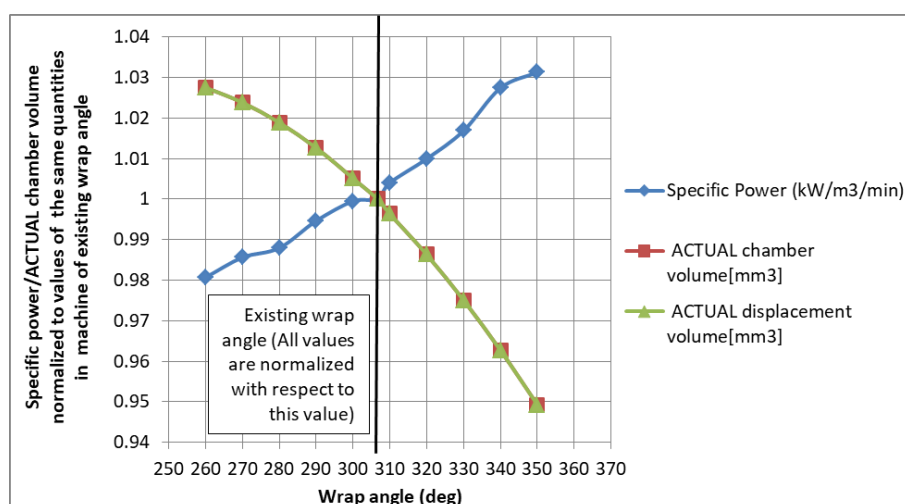


Figure 4.14: Variation in actual chamber volume and actual displacement volume with respect to wrap angle.

Built-in volume ratio:

The built-in volume ratio, defined as the ratio of the suction volume to the discharge volume, significantly influences compressor performance. A higher VI can enhance the discharge flow rate but also leads to greater leakage and friction, increasing power consumption and reducing efficiency.

For a pressure ratio of 8.5, an optimal VI of 4.6 provides the best balance (see Figure 4.15). Deviations from this value result in performance losses due to mismatched internal and external pressures:

- **Under-compression** ($VI < 4.6$): When VI is below 4.6, internal compression does not fully meet the external pressure ratio, resulting in under-compression. This mismatch requires additional external compression, increasing SPC.
- **Over-compression** ($VI > 4.6$): Conversely, a VI above 4.6 leads to over-compression, where the discharge pressure exceeds the external discharge pressure. This excess pressure increases leakage losses and friction, further raising SPC.

Therefore, a VI of 4.6 aligns internal and external pressures optimally, minimizing both under and over-compression losses and enhancing compressor efficiency.

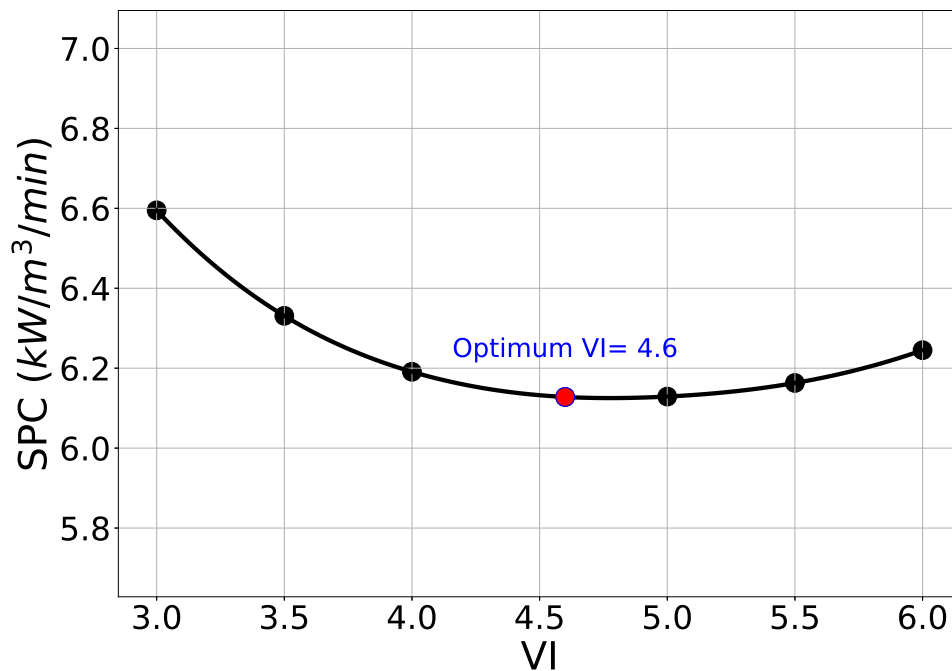


Figure 4.15: Influence of built-in volume ratio on screw compressor performance at a pressure ratio of 8.5.

Effect of fluid injection parameters on compressor performance:

The fluid injection parameters play a critical role in influencing specific power consumption and discharge temperature in screw compressors.

Oil injection pressure:

As illustrated in Figure 4.16, increasing oil injection pressure enhances the oil quantity within the compressor. This additional oil improves sealing efficiency, thereby reducing leakage and lowering discharge temperature due to enhanced cooling effects. However, the increase in oil quantity also results in greater oil drag, which contributes to higher SPC. Therefore, an optimal balance must be maintained to maximize performance.

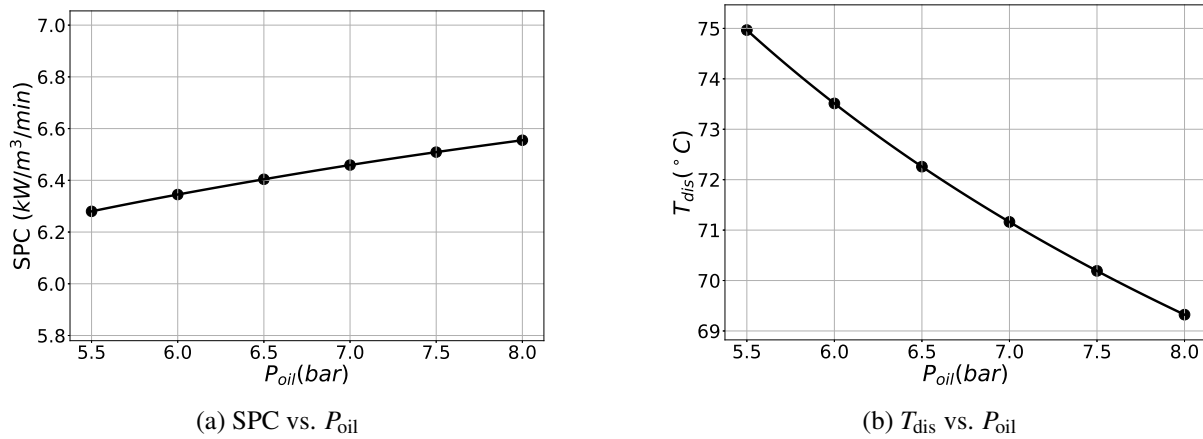


Figure 4.16: Effect of oil injection pressure on specific power consumption and discharge temperature at a pressure ratio of 8.5.

Oil injection port diameter:

Figure 4.17 indicates that the oil injection port diameter significantly affects performance. A smaller diameter restricts oil flow, leading to insufficient sealing and higher SPC. Conversely, a larger diameter increases oil flow, but this results in greater oil drag, which also elevates SPC. Therefore, an optimal oil port diameter, typically around 5 mm, is crucial for balancing flow and drag.

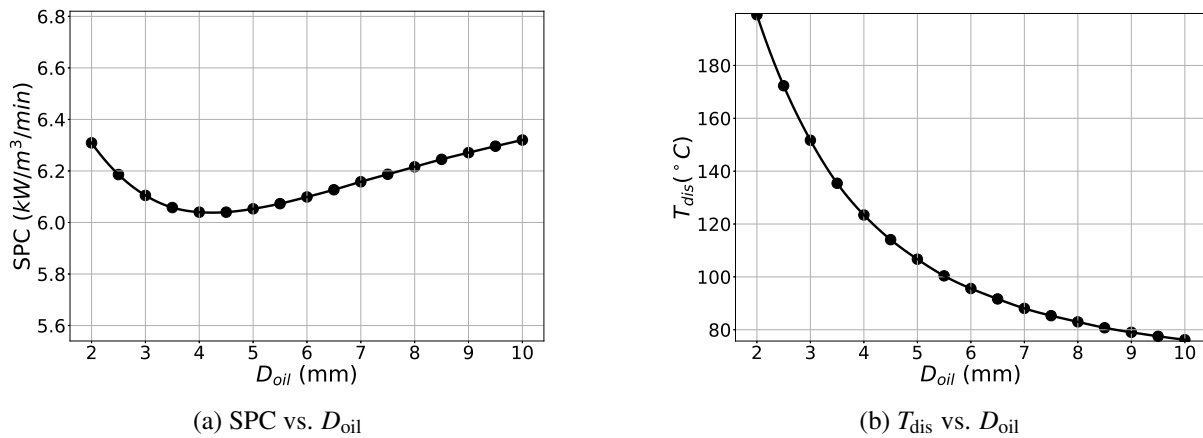


Figure 4.17: Effect of oil injection port diameter on specific power consumption and discharge temperature at a pressure ratio of 8.5.

Oil injection temperature:

Figure 4.18 demonstrates that lower oil injection temperatures enhance SPC by absorbing more heat from the compression chamber, thus improving thermal efficiency and lowering discharge temperatures. However, maintaining lower temperatures places a higher load on the oil cooler, increasing overall power consumption. An optimal injection temperature range of 40 to 60 °C is recommended to balance cooling efficiency and energy demands.

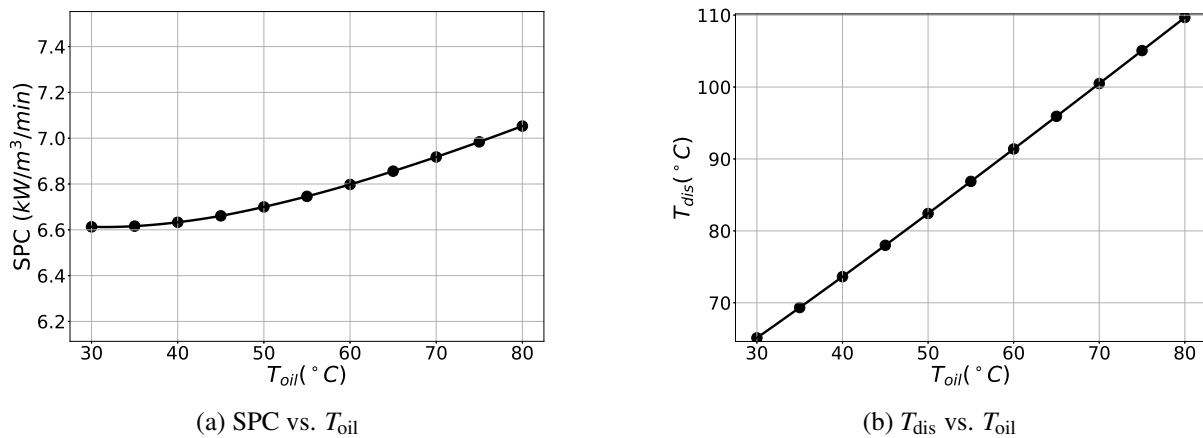


Figure 4.18: Effect of oil injection temperature on specific power consumption and discharge temperature at a pressure ratio of 8.5.

Oil injection angle:

The oil injection angle significantly impacts the location and effectiveness of oil distribution within the compression chamber. A lower angle positions the injection closer to the suction side, increasing residence time and drag power. Conversely, an excessively high angle near the discharge port reduces residence time, limiting heat transfer and adversely affecting performance (see Figure 4.19). For optimal performance, an oil injection angle between 60° and 90° is recommended, striking a balance between effective heat transfer and reduced drag.

The experimental results align with SCORG simulation outcomes, highlighting the following trends:

- Water injection reduces SPC and discharge temperatures.
- Increasing rotor speed improves flow rate but elevates SPC.

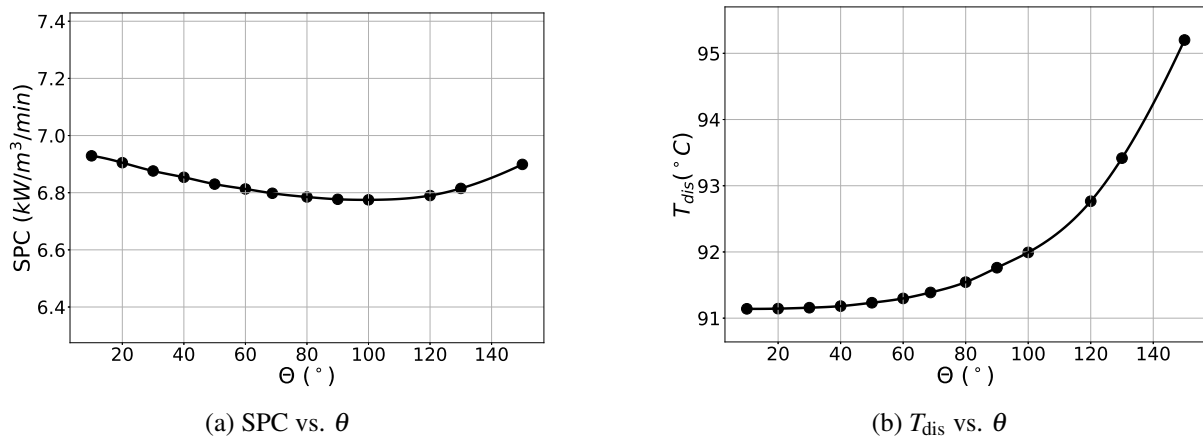


Figure 4.19: Effect of oil injection angle on specific power consumption and discharge temperature at a pressure ratio of 8.5.

- Optimal VI minimizes compression losses.

These findings provide essential insights into the influence of design parameters and fluid injection on screw compressor performance, establishing a foundation for future optimization studies.

4.7 Case Studies on optimisation: Evolutionary and Bayesian approaches

4.7.1 Optimisation using Evolutionary algorithms

The subject of this study is a 22 kW air screw compressor, designed with a built-in volume ratio of 4.6, operating at a pressure ratio of 8.5, and a speed of 2000 rpm. This compressor, manufactured at KPCL, is an industrial-grade screw compressor. Table 4.6 presents the normalized performance data of the compressor block, offering a visual representation of performance improvements achieved through optimisation. Experimental testing has been carried out on this compressor, with the collected data forming the foundation for modeling in the SCORG software.

For multi-objective optimisation in this work, the weighted-sum design approach has been adopted. Equal weights are assigned to each objective function, ensuring all outputs are given equal importance. This approach simplifies comparisons across different optimisation algorithms and ensures a balanced evaluation of performance metrics.

Input and output functions

In air screw compressors, as the pressure increases, the temperature within the compression chamber also rises significantly. For instance, in an oil-free twin screw compressor operating at a pressure ratio of 6 and approximately 6000 rpm, the average discharge temperature can exceed 320°C. Oil injection plays a crucial role in mitigating this temperature rise by cooling the compression chamber, improving volumetric efficiency through sealing of leakage gaps, and providing lubrication for rotors and bearings [4].

In screw compressor industries, a general guideline is that oil contributes to cooling, sealing, and lubrication in a mass ratio of 100:10:1, respectively. While oil injection has clear advantages, the quantity must be carefully optimized. Excessive or insufficient oil injection can result in power losses, adversely affecting compressor performance.

Input parameters and their effects: For optimisation, the following input parameters are considered as they directly influence the compressor's performance:

- **Oil port diameter (mm):** Determines the oil flow rate, which impacts the heat exchange between gas and oil. While higher oil flow rates reduce discharge temperature and improve volumetric and adiabatic efficiencies, excessive flow can cause power losses due to the high density of oil compared to gas.
- **Oil injection angle (°):** The positioning of the oil injection port significantly affects the heat transfer. If the port is located near the discharge side, the reduced residence time limits heat exchange. Optimal positioning ensures effective cooling without excessive losses.
- **Oil injection temperature (°C):** Lower injection temperatures improve heat exchange but may increase the cooling system load. An optimal balance must be achieved to maintain efficiency.
- **Pressure in oil reservoir (bar):** Higher reservoir pressure reduces oil droplet size, increasing surface area for heat exchange and enhancing cooling efficiency.
- **Oil viscosity (m^2/s):** Low viscosity can lead to metal-to-metal contact, causing component failure, while high viscosity reduces operational efficiency and increases power losses. Optimal viscosity ensures both lubrication and efficiency.

The combined effect of these parameters governs the temperature within the compression chamber, which directly impacts the compressor's performance. Table 4.3 summarizes the range of these input parameters for typical screw compressor operations.

Optimisation objectives: The output functions used for multi-objective optimisation are the performance metrics as described in Appendix B.

For single-objective optimisation, the focus is on minimizing specific power consumption (SPC), ensuring energy-efficient operation of the oil-injected screw compressor.

Range of input parameters: The input parameters considered in this study, along with their ranges, are presented in Table 4.3:

Table 4.3: Range of Input Parameters

Input Parameter	Range
Oil Port Diameter (DIOIL)	1–12 mm
Oil Injection Angle (FIOIL)	35°–130°
Oil Injection Temperature (TOIL)	35–80°C
Oil Reservoir Pressure (POIL)	3.5–8 bar
Oil Viscosity (VISCOIL)	$(1–8) \times 10^{-6} \text{ m}^2/\text{s}$

By carefully tuning these input parameters, this work aims to optimize compressor performance while ensuring energy-efficient operation. The results of this optimisation demonstrate significant improvements in flow rate, SPC, and overall efficiency.

Single-objective optimisation

The simulation results from the GT-SUITE_SCORG model are presented in this section. In the single-objective optimisation using the different evolutionary algorithms, a comparative analysis has been presented. An important thing to note is that all the different algorithms for optimisation are simulated independently with the same input range for variables and the same objective function. For a single objective optimisation the specific power consumption is considered. The input parameters are the same for both the multi-objective and single-objective optimisation so that a proper conclusion can be obtained and the results are validated.

From Figure 4.20 it can be seen that the change in specific power consumption for GA is around 10.8 % , for simplex is 10.5%, for CMA-ES is 9.6% and for accelerated GA is 9.2% respectively.

The time elapsed for each search algorithm is shown in Figure 4.21. Simplex method takes the least time whereas the GA takes the highest time for single objective optimisation.

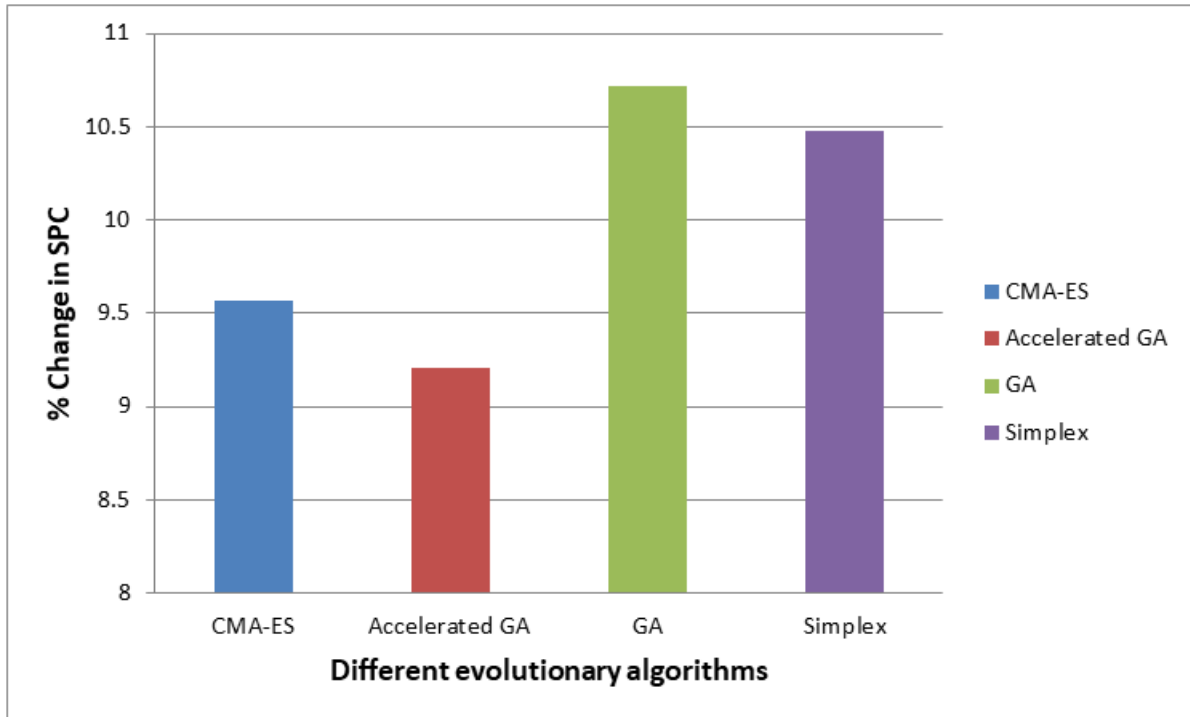


Figure 4.20: % Change in SPC (Single-objective optimisation)

Multi-objective optimisation

In this section, a comparative analysis using the different evolutionary algorithms are presented for each objective function. Figure 4.22 shows the percentage change in specific power consumption for different algorithms with GA showing the highest variation of 10.8% and the accelerated GA with the lowest of 9.2% which is validated from single-objective optimisation.

It is also evident from Figure 4.23 and 4.24 that the change in flow and the volumetric efficiency is maximum for GA and the least for accelerated GA. Apart from the thermodynamics performance analysis a comparative study of the elapsed time is also presented in Figure 4.25. Here, it can be seen that the simplex search algorithm takes the least time for multi-objective

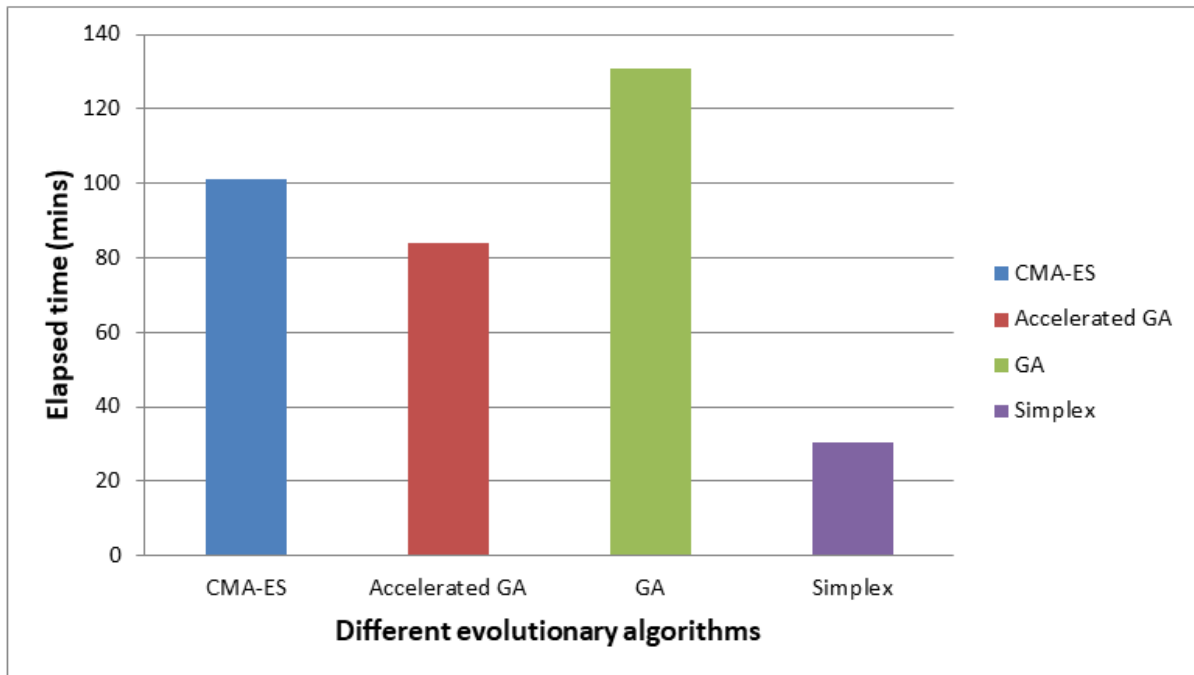


Figure 4.21: Time elapsed for single-objective optimisation

optimisation and the GA takes the highest time for predicting the optimum output. This depends on the step-length and the seed size taken during the optimisation.

The seed size taken here for optimisation using the evolutionary algorithms for both the single-objective and multi-objective are listed below in the table-4.4.

Table 4.4: Seed Size for Optimisation

Search Algorithm	Seed Size
GA	0.033005270
CMA-ES	0.10439938
Accelerated GA	0.24159176

Table 4.5: Optimisation parameters used for different evolutionary algorithms

Algorithm	Population Size	Generations	Mutation Rate	Crossover Rate
Genetic Algorithm (GA)	50	100	0.01	0.8
Accelerated GA (AGA)	50	100	Adaptive	Adaptive
CMA-ES	30	150	N/A	N/A

The fitness function determines how fit an individual is, essentially, its ability to compete

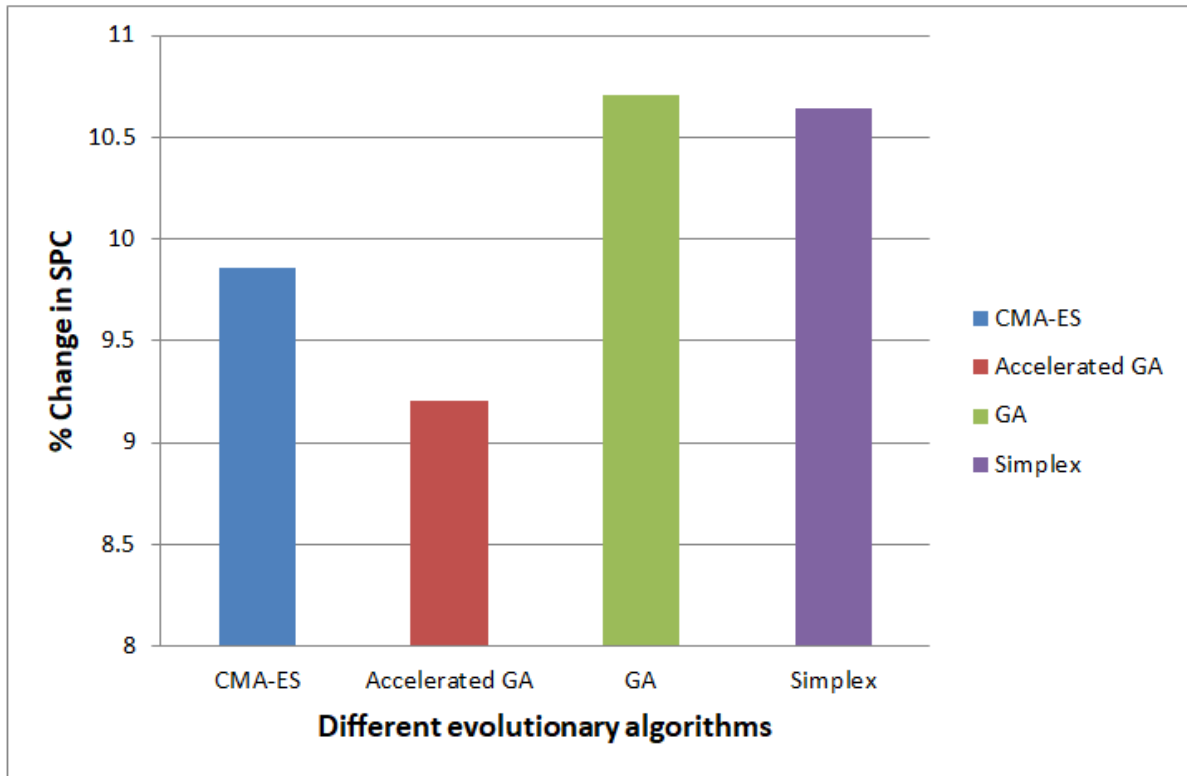


Figure 4.22: % Change in SPC (Multi-objective optimisation)

with other individuals in the optimisation process. It assigns a fitness score to each solution candidate, with higher scores corresponding to better-performing solutions. In this study, functions with higher fitness values are preferred, and fitness is inversely proportional to seed size, meaning that a smaller seed size yields a higher fitness value. Based on this criterion, the GA exhibits the highest fitness score, followed by CMA-ES and then the Accelerated GA (AGA).

To ensure transparency and fairness in algorithm comparison, the optimisation parameters used for each evolutionary algorithm are summarised in Table 4.5. While these algorithms inherently differ in their exploration-exploitation strategies and internal heuristics, a consistent cap of 1000 function evaluations was enforced across all methods. This uniform evaluation budget eliminates bias and reflects practical computational limitations when using expensive simulations like those in GT-SUITE. Notably, CMA-ES adaptively updates its covariance matrix using previous samples, enabling it to explore complex, high-dimensional landscapes more effectively. In contrast, classical GA and AGA rely on probabilistic population-based operators, which, although versatile, may converge prematurely in rugged objective spaces.

Due to GT-SUITE's current constraints, convergence traces (i.e., fitness vs. iterations)

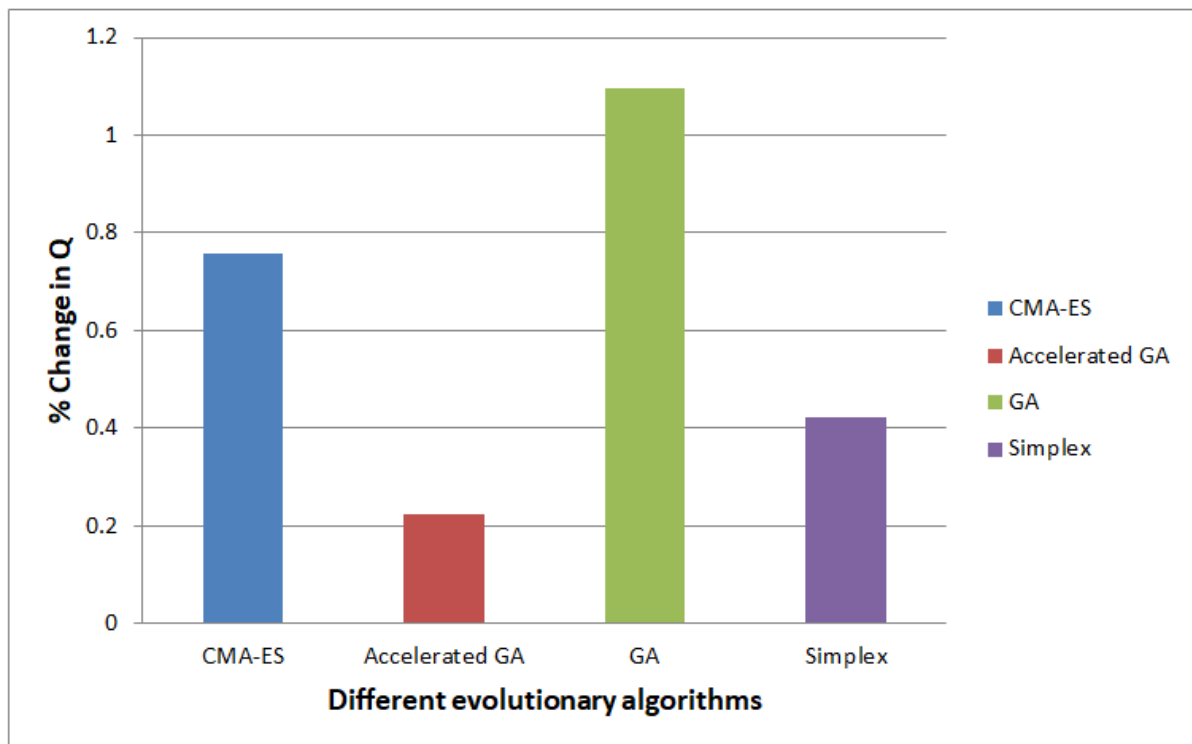


Figure 4.23: % Change in Q (Multi-objective optimisation)

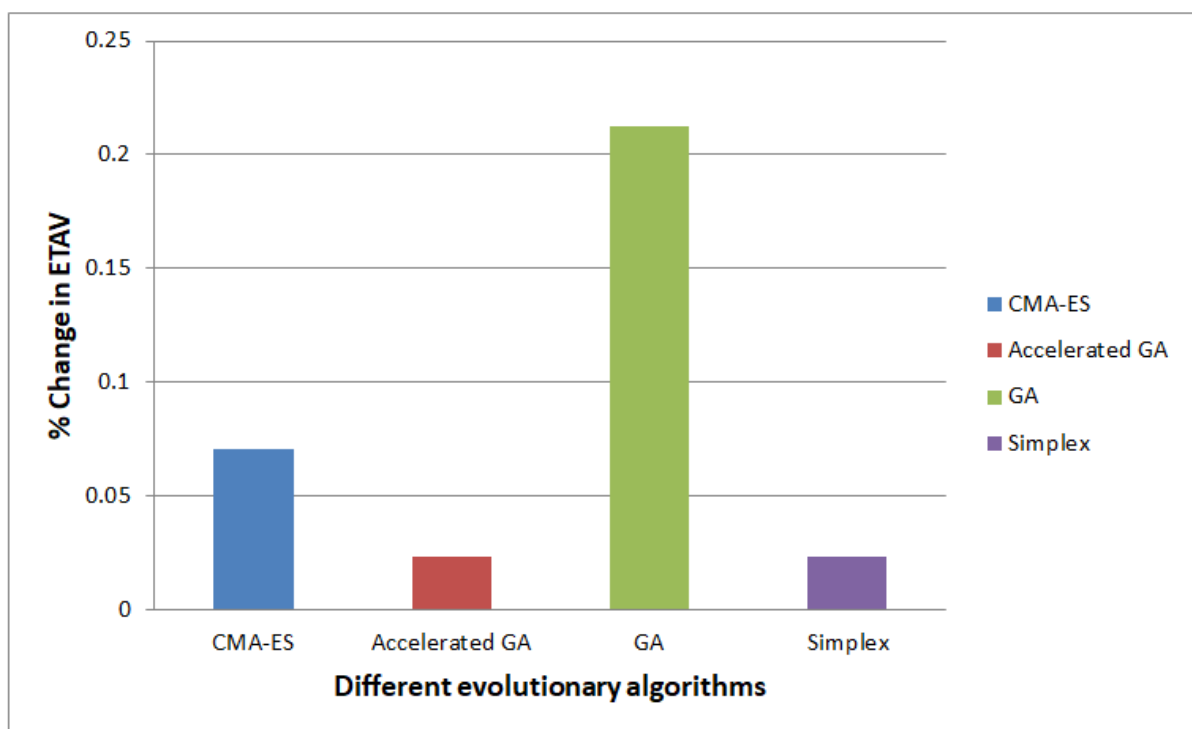


Figure 4.24: % Change in ETAV (Multi-objective optimisation)

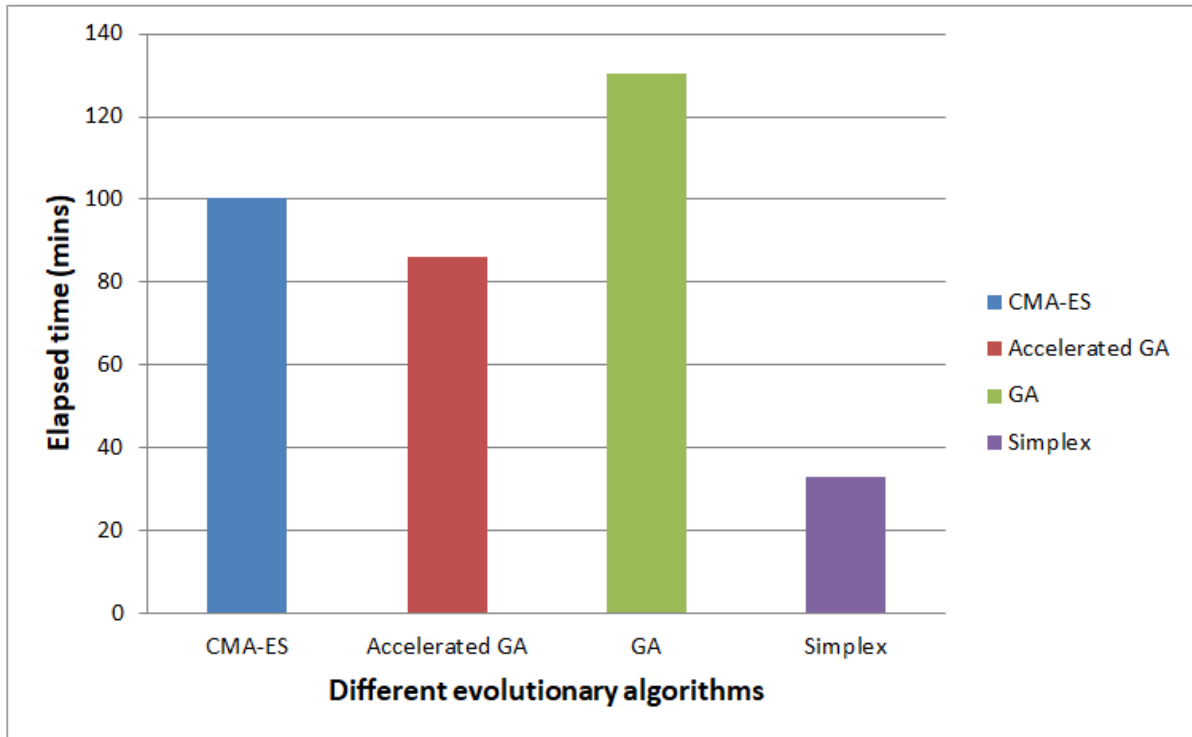


Figure 4.25: Time elapsed for multi-objective optimisation

were not directly extractable. However, to mitigate the risk of local optima and to enhance robustness, each optimisation algorithm was executed for multiple independent runs using identical initial settings, and the best-performing result was selected for comparison. This approach reduces stochastic variability and provides a fair basis for evaluating performance across methods.

It is important to clarify that the primary objective of this comparative study is not to establish a definitive ranking of optimisation algorithms, but to evaluate their applicability and behaviour when applied to real-world compressor design problems. These insights inform the later adoption of Bayesian Optimisation, which addresses certain limitations observed in evolutionary algorithms, including sensitivity to local optima and the high computational expense associated with iterative simulation-based evaluations.

The normalized performance map after the optimisation is shown in table-4.6 in comparison to the original KPCL model of screw compressor. The specific power consumption is normalized with the one having the minimum value and the remaining two i.e flow and volumetric efficiency are normalized with the one having the maximum value. These results highlight the capability of each algorithm to enhance different aspects of compressor performance, with

Table 4.6: Normalized Performance Map

Model	SPC	Q	ETAV
KPCL Model	1.120	0.989	0.998
CMA-ES	1.009	0.997	0.999
Accelerated GA	1.017	0.991	0.998
GA	1.000	1.000	1.000
Simplex	1.001	0.993	0.998

Genetic Algorithm providing the most balanced outcome under the defined fitness criteria.

On account of the optimisation performed here, the optimum parameters obtained from any of the evolutionary algorithms shows that they are almost in the same range such as optimum oil injection angle being in the range of $(40-65)^\circ$, the oil injection temperature in the range of $(30-40)^\circ\text{C}$, the oil port diameter in the range of $(6-7)$ mm, pressure in the oil reservoir in the range of $(5-6.5)$ bar and the oil viscosity in the range of $(1-2)*10^{-6} \text{ m}^2/\text{s}$. This signifies that injecting oil at a lower temperature with lower oil viscosity and injecting earlier will result in improvement of performance by more than 5% as it will lead to near isothermal efficiency which is indeed a good choice of compressor. Thus from the screw compressor block point of view these optimum parameters are the best suited ones.

However, from the system design point of view there are other important conditions which need to be incorporated as constraints to the optimisation algorithms for reliable performance of the compressor.

For better understanding a sensitivity analysis has been shown in figure-4.26 to understand the effect of parameters on the objective functions. The analysis clearly shows that the major parameters which are contributing to the significant amount of change in the performance of the 22 kW twin screw air compressor are the oil viscosity followed by the oil injection temperature.

To achieve an improvement in specific power, the oil viscosity must be significantly reduced. However, there is a limitation on how much the viscosity can be lowered while ensuring smooth bearing operation, feasible bearing life, and adequate film formation for bearing lubrication. According to the bearing manufacturer, the viscosity ratio, or kappa value, must be greater than or equal to one for proper bearing function. Kappa is defined as the ratio of the actual oil viscosity to the minimum viscosity required to support a dynamic load within a

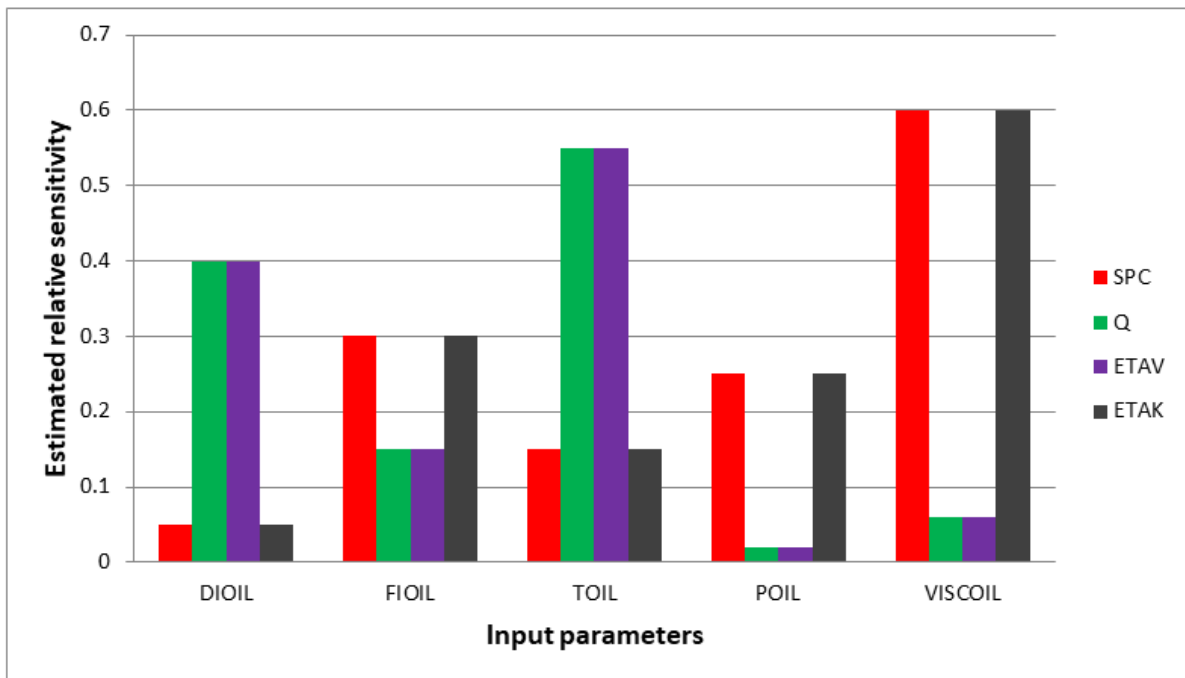


Figure 4.26: Sensitivity comparison for output vs. input

bearing for full film lubrication. In the current KPCL model, the kappa value is already at the lower limit specified by the manufacturer, indicating that reducing oil viscosity further is not recommended from the bearings' perspective.

In addition, a lower oil injection temperature is desirable from the compressor block's standpoint as it improves the block's thermal performance. However, from a system design perspective, a lower oil injection temperature increases the temperature difference between the compressor's inlet and outlet. The desirable discharge temperature for the compressor is in the range of 80 – 90°C. Increasing the temperature difference amplifies the heat load on the cooling unit, which is a critical factor in system-level optimisation. As a result, the optimum oil injection temperature should lie within the range of 40 – 60°C, balancing the requirements of the compressor block and the system as a whole.

The optimisation of a 22 kW oil-injected twin-screw air compressor was performed using various evolutionary algorithms. The SCORG model demonstrated strong agreement with experimental results and was seamlessly linked to the GT-SUITE model for optimisation. A GT-Process Map was created using the GT-ISE interface, with SCORG providing thermodynamic calculations in the background. Key oil parameters were used as inputs, while performance metrics such as specific power consumption, adiabatic efficiency, volumetric efficiency, and

flow served as outputs. A comparative analysis revealed that the simplex algorithm achieved the fastest convergence while delivering optimal parameters comparable to other algorithms. Meanwhile, the Genetic Algorithm (GA) outperformed in handling medium to high complexity problems, achieving the smallest seed size and highest fitness value. These findings underscore the effectiveness of the proposed optimisation framework in improving screw compressor performance, while highlighting the importance of balancing oil parameters to meet both block-level and system-level requirements.

4.7.2 Optimisation using Bayesian framework: Weighted-sum approach

The study aims to optimise the KAS-300 compressor block, a gear-driven, oil-flooded screw compressor with a 22 kW power rating. This compressor features a built-in volume ratio of 4.6 and is designed to operate at pressure ratios of 7.5, 8.5, 10, and 13, with tip speeds ranging from 15 to 45 m/s. Experimental testing of the KAS-300 compressor block was carried out at the Centre for Compressor Technology, City, University of London [50]. The obtained data was used to create a digital model of the KAS-300 in SCORG software [9], which serves as the physics solver for optimisation. This SCORG-enhanced KAS-300 model is employed for the thermodynamic calculations needed in the chamber model optimisation process [62].

Input functions

The developed optimisation framework targets profile clearances, which are crucial for the performance of screw compressors. This study focuses on optimising three essential profile parameters:

1. Interlobe Clearance (GAPI) in μm : This parameter refers to the space between the male and female rotor lobes, making it a critical parameter. A smaller interlobe clearance reduces gas leakage, improving volumetric and adiabatic efficiency. However, excessively small clearances can result in rotor contact, potentially causing damage and reducing the compressor's lifespan.
2. Radial Clearance (GAPR) in μm : This parameter determines the distance between the rotor lobes and the compressor housing, affecting gas leakage and friction within the compressor.

3. Axial Clearance (GAPA) in μm : This parameter determines the distance between the rotor lobes and the compressor housing in the axial direction, influencing gas leakage and friction within the compressor.

The range of input parameters for optimisation, representative of typical screw compressor operating conditions, is presented in Table 4.7.

Table 4.7: Optimisation bounds for input variables

Profile Parameters	Bounds
GAPI	(10 - 150) μm
GAPR	(10 - 150) μm
GAPA	(10 - 150) μm

Effect of input variables on objective functions

To optimise the performance of the screw compressor, it is essential to understand the impact of input variables on the objective functions. Figure 4.10 illustrates the effect of profile clearances on the performance of the screw compressor under a pressure ratio of 8.5. As shown in the figure, as clearances increase, compressor performance decreases. This is primarily attributed to two key factors:

- Increased gas leakage: Larger clearances permit more gas to escape between the rotor lobes and the compressor housing. This reduces the trapped and compressed gas, resulting in lower volumetric efficiency.
- Increased turbulence and friction: Larger clearances can also lead to heightened turbulence and friction within the gas flow, diminishing the adiabatic efficiency of the compressor.

As clearances increase, compressor performance decreases. However, excessively reducing clearances, leads to exponential performance deterioration. Lower clearances increase oil drag and may cause wear and tear, potentially impacting the compressor's reliability and longevity.

These factors underscore the importance of optimising profile clearances to achieve optimal compressor performance.

Optimisation comparison

This section provides a detailed comparison of the optimisation algorithms evaluated in this study, summarized in Table 4.8. The table showcases the performance outcomes for Bayesian Optimisation, Nelder-Mead, Powell, Particle Swarm Optimisation (PSO), and Evolutionary Optimisation using a Genetic Algorithm (GA). Each algorithm's performance is measured as a percentage change relative to the baseline KAS-300 compressor performance, which is presented without optimisation. The sign in the tabular column indicates the direction of change in performance parameters compared to the KAS-300 (Baseline) with no optimisation. A negative sign indicates a deterioration in performance, while a positive sign indicates an improvement. This notation helps to quickly identify the impact of optimisation on key performance metrics, such as flow, power consumption, and specific power consumption.

Table 4.8: Comparative analysis for profile parameters optimisation

Algorithms	Optimal Clearances (μm)	Q (%)	P (%)	SPC (%)	Time Duration (s)
KAS-300 (Baseline)	(70, 70, 70)	-	-	-	-
Bayesian	(15, 46, 52)	58.34	-5.78	33.19	195
Nelder-Mead	(12, 42, 33)	64.31	-5.35	35.88	845
Powell	(94, 94, 94)	-29.48	0.64	-40.88	67
PSO	(104, 88, 101)	-35.82	2.05	-52.61	55
BFGS	(60, 60, 60)	12.43	-0.33	10.76	1039
Evolutionary (GA)	(14, 44, 43)	60.72	-5.48	34.38	9450

The results of this study indicate that Bayesian Optimisation consistently achieves the optimal solution in the shortest time frame with the fewest iterations, making it a highly efficient method for performance optimisation. This is followed by the Nelder-Mead algorithm, which, while effective, requires more time and iterations to converge to the optimal solution. In contrast, Powell and Particle Swarm Optimisation (PSO) algorithms demonstrated negative improvements, with Powell's performance hindered by slow convergence in high-dimensional spaces, potentially leading to local minima. Similarly, PSO exhibited premature convergence, resulting in suboptimal solutions; however, tuning its hyperparameters could enhance its performance, particularly when applied to screw parameter optimisation using the Machine Learning-based solver.

The Evolutionary framework, employing a Genetic Algorithm (GA), achieved optimal parameters with approximately a 35% improvement in Specific Power Consumption (SPC). However, the time required for Evolutionary optimisation was longer compared to the Bayesian

framework algorithms. A detailed view of the optimisation process, including the objective function versus the number of iterations, is shown in Figure 4.27, which compares the performance of various algorithms.

Bayesian Optimisation stands out as a compelling alternative to conventional methods due to its computational efficiency and ability to obtain near-optimal solutions with minimal iterations. The framework developed in this study integrates the chamber model for comprehensive performance optimisation of screw compressors, accommodating a wide range of input parameters, including design, geometrical, and fluid-related parameters. The effectiveness of this approach was validated through two distinct case studies. The first focused on optimising profile parameters, as detailed in this work, while the second, presented in Kumar et al. [50], explored the optimisation of design parameters for the KAS-300 industrial compressor model. In both scenarios, Bayesian Optimisation demonstrated superior computational efficiency and reduced computational effort compared to conventional methods, highlighting its robustness and versatility as a tool for advancing screw compressor performance.

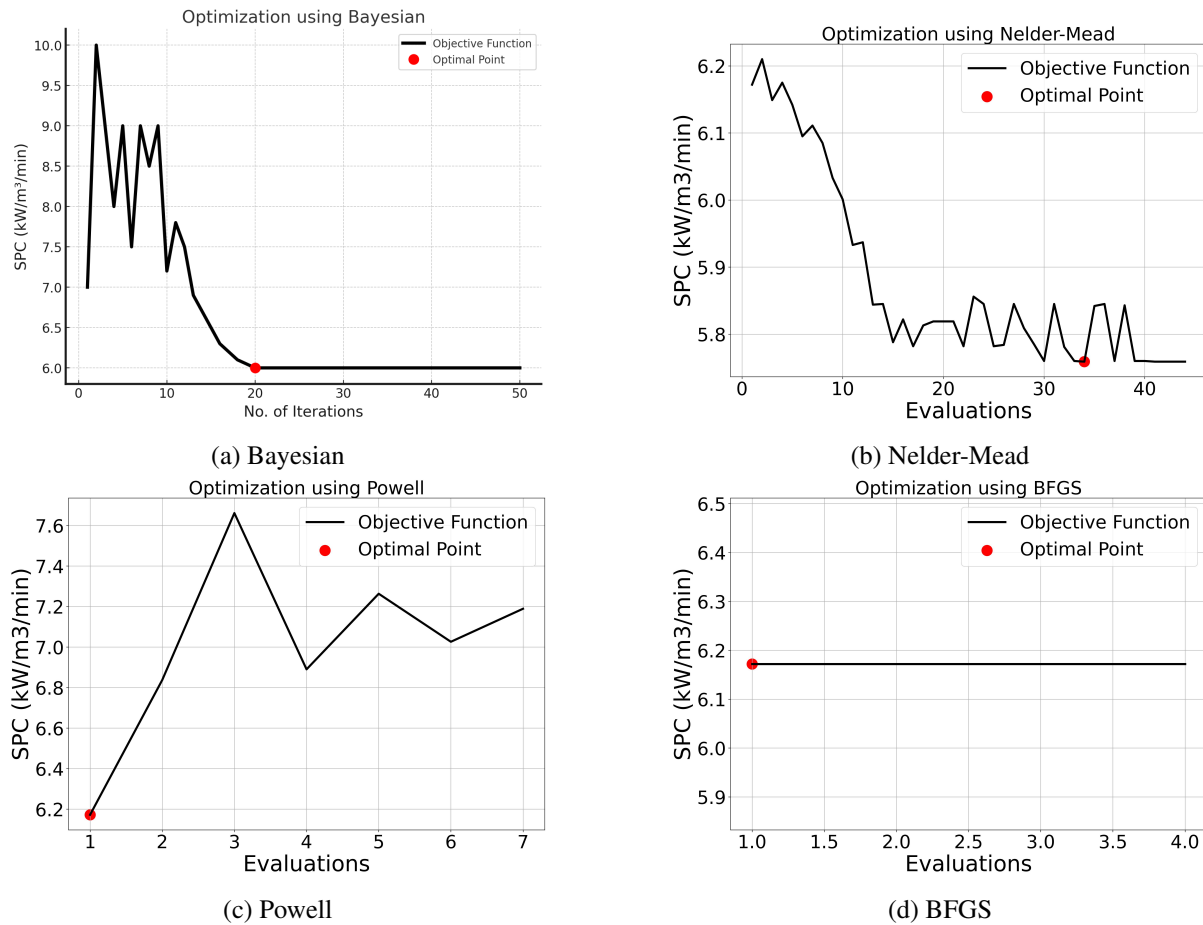


Figure 4.27: Objective Function vs. Number of Iterations

4.7.3 Optimisation using Bayesian framework: Pareto analysis

This section details the Pareto optimization of the KAS-300 screw compressor block using the Bayesian framework. The optimization aimed to minimize power consumption while maximizing flow rate by adjusting key input variables. The compressor block specifications and initial SCORG simulation results are as follows:

- **Compressor Block:** KAS-300
- **Power Rating:** 30 kW
- **Pressure Ratio:** 7.5
- **Original Power (Before Optimization):** 34.499 kW
- **Flow (Before Optimization):** $5.725 \text{ m}^3/\text{min}$

- **Speed of Male Rotor:** 3261 RPM

The optimization considered the following input variables:

- Oil Injection Pressure (**POIL**)
- Oil Injection Temperature (**TOIL**)
- Oil Injection Angle (**FIOIL**)
- Oil Injection Diameter (**DOIL**)

The objectives of the optimization were:

- **Minimize:** Power consumption
- **Maximize:** Flow rate

The parameter bounds and initial values used in the optimization are summarized in Table 4.9.

Table 4.9: Parameter Bounds and Initial Values for Pareto Optimization

Parameter	Lower Bound	Upper Bound
Oil Injection Pressure (POIL) [Pa]	500,000	800,000
Oil Injection Temperature (TOIL) [K]	313.15	363.15
Oil Injection Angle (FIOIL) [rad]	0.5	2.5
Oil Injection Diameter (DOIL) [m]	0.005	0.02

The optimization was carried out using the chamber model coupled with Bayesian Framework. The Pareto front obtained from the Bayesian framework presents optimized solutions for the given objectives. The total elapsed time for the optimization process was approximately 34714.09 seconds. Table 4.10 highlights a selection of key Pareto-optimal points:

Figure 4.28 shows the Pareto front visualization, demonstrating the trade-off between minimizing power and maximizing flow.

The Pareto analysis reveals a set of optimal solutions, allowing the decision-maker to balance conflicting objectives effectively. The Bayesian framework proves to be a robust tool for optimizing performance parameters of screw compressors, achieving a comprehensive understanding of trade-offs between key objectives.

Table 4.10: Pareto-Optimal Results for KAS-300 Compressor Block

Point	POIL (Pa)	TOIL (K)	FIOIL (rad)	DOIL (m)	Power (kW)	Flow (m^3/min)
1	778,125.0	313.15	1.2450	0.0104	36.689	5.777
2 (Optimal)	767,798.0	332.76	1.1835	0.0099	28.069	7.627
3	500,000.0	336.65	1.4200	0.0103	177.874	9.589
4	800,000.0	313.15	1.2431	0.0100	134.154	9.952
5	800,000.0	313.15	1.2431	0.0100	134.154	9.952

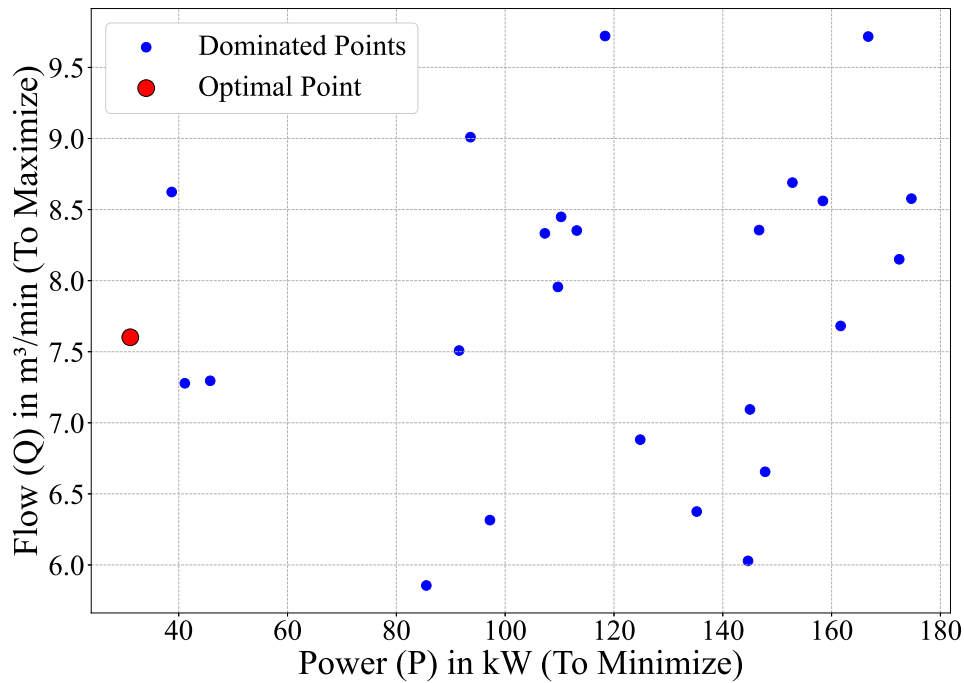


Figure 4.28: Pareto Front for Multi-Objective Optimization of KAS-300 Compressor Block.

4.8 Summary

This chapter introduced two innovative optimization frameworks—Evolutionary and Bayesian—tailored to enhance the performance of screw compressors. The Evolutionary Framework leverages advanced algorithms, such as the Genetic Algorithm (GA), to optimize thermodynamic performance through iterative exploration of design parameters. Complementing this, the Bayesian Framework integrates machine learning techniques like Gaussian Process Regression (GPR) with traditional chamber models to improve computational efficiency and accuracy in solving single- and multi-objective optimization problems.

Key findings revealed that Bayesian Optimization achieved optimal results with minimal iterations and computational time, outperforming other methods like Nelder-Mead, Powell, and

Particle Swarm Optimization (PSO). Evolutionary algorithms, while robust, required longer timeframes, particularly for high-complexity problems. A weighted-sum approach and Pareto analysis highlighted the trade-offs between conflicting objectives, offering optimal solutions for flow rate, power consumption, and specific power consumption (SPC). Experimental and simulation-based analyses demonstrated that profile clearances, fluid injection parameters, and geometrical characteristics significantly impact compressor performance. For instance, water injection improved energy efficiency and reduced SPC compared to oil injection, albeit with challenges like corrosion and scaling.

Through a combination of experimental validation and computational modeling using SCORG and GT-SUITE, the frameworks successfully optimized key design parameters, achieving performance improvements of up to 35%. These advancements underline the potential of integrating physics-based and machine learning-driven approaches to tackle complex optimization challenges, providing a robust foundation for future compressor designs and system-level optimizations.

Chapter 5

Modelling Framework for Multi-Stage Screw Compressors

5.1 Introduction

This chapter presents a comprehensive framework for the prediction and optimisation of screw compressor performance, integrating traditional chamber models with advanced Machine Learning (ML) techniques. The research initially focuses on single-stage screw compressors and extends its scope to the optimisation of industrial oil-flooded compressors, utilizing Bayesian Optimisation as the core optimisation engine. The methodology, while tailored to specific compressor configurations, demonstrates significant potential for generalization across various sizes, designs, and multi-stage applications.

In this study, Gaussian Process Regression (GPR) emerged as the most accurate and robust ML model for performance prediction among the techniques explored, including Support Vector Machines, Artificial Neural Networks, and polynomial regression. The inherent uncertainty quantification capability of GPR further reinforces its suitability for thermodynamic modeling. To enhance the performance of the GPR model, Bayesian Optimisation was employed to fine-tune its hyperparameters. This probabilistic optimisation technique leverages surrogate models of the objective function to balance exploration and exploitation, efficiently navigating the optimisation landscape.

The proposed hybrid framework combines the precision of traditional chamber models with the adaptability and computational efficiency of Machine Learning. This integration enables accurate performance prediction and optimisation while reducing computational effort. The framework's application to a two-stage air screw compressor demonstrated its capability to predict performance within a 5% error margin, underscoring its reliability for high-pressure and multi-stage configurations.

By adopting this advanced modeling approach, the study highlights a paradigm shift in screw compressor technology, prioritizing data-driven methodologies to enhance efficiency,

reduce energy consumption, and improve reliability. This chapter lays the groundwork for further research into scalable, adaptive, and versatile modeling tools that address the complex challenges of modern screw compressor design and optimisation.

5.2 Machine Learning-based performance prediction and optimisation

5.2.1 Dataset generation

To effectively train a machine learning model, a large number of datasets are usually necessary depending on the application and the range of parameters involved. However, the acquisition of such a substantial dataset from experimental testing is often unfeasible. To address this challenge, a validated physics-based screw compressor model was developed and utilised in the present study. The screw compressor was modeled using SCORG (Screw Compressor Rotor Grid Generation) software from PDM Analysis, a leading grid generation and performance software for positive displacement screw machines. SCORG performs thermodynamic calculations based on a multi-chamber model, employing conservation equations of mass and internal energy for control volumes [9, 1]. The screw compressor considered in this study is the KAS-300 oil-flooded air screw compressor (gear-driven) with a built-in volume ratio of 4.6, operating at pressure ratios of 6.5, 8.5, 10.5, and 12.5, with a tip speed ranging from 15 to 45 m/s. It is manufactured by Kirloskar Pneumatic Company Limited in Pune, India. Due to its commercial nature, detailed information about the compressor's size and profile cannot be disclosed. Experimental testing for this compressor was conducted at the Centre for Compressor Technology, City University of London, and the obtained data was used for validating the screw compressor model in SCORG.

After setting up the SCORG model for this compressor configuration, a batch file was linked with the programming language, Python to automate the data generation framework. Four key design variables were selected to be varied within the data generation framework, and their respective ranges and step lengths are provided in the accompanying Table 5.1. This approach facilitated the generation of an extensive dataset comprising 24,000 individual instances.

For data set visualization, heatmaps were generated, as shown in Figure 5.1. The output parameters encompass key performance metrics crucial in screw compressor applications: Power Consumption (P), Volume Flow Rate (Q), Volumetric Efficiency (ETAV), and Adiabatic

Table 5.1: Input Parameter Variations for Data Sets Generation

Input Parameters	Range	Step Length	No. of Instances
W_{tip} (m/s)	(15, 50)	0.7	50
VI	(2.1, 5.1)	0.5	6
L/D	(0.5, 2.5)	0.5	4
ϕ (rad)	(3.8, 7)	0.16	20
Total no. of data sets			24,000

Efficiency (ETAK), collectively shaping the compressor's operational effectiveness and energy efficiency. These heatmaps present the correlations among the input variables and output parameters in the dataset. Brighter colors indicate more pronounced positive or negative correlations, while darker colors suggest weaker or negligible correlations. It can be observed that the heatmap provides valuable insights into the interrelationships between the variables, which helps further in model development and enhances the overall interpretability of the machine learning model.

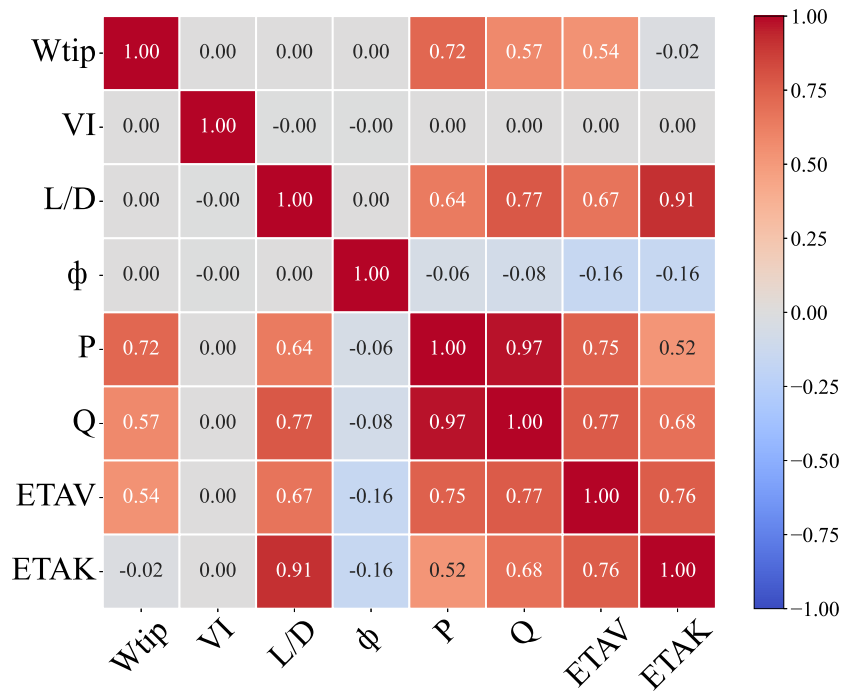


Figure 5.1: Correlation Heatmaps for input and output Parameters

5.2.2 Model development

Model architecture

Gaussian Process Regression (GPR) [69] is utilized as the primary governing machine learning model in this study. Unlike conventional regression techniques, GPR does not assume fixed functional forms for the data, rendering it suitable for handling complex and non-linear relationships. The underlying concept of GPR relies on Gaussian processes and collections of random variables. The target variable is modelled as a multivariate Gaussian distribution, where the mean function represents the underlying trend, and the covariance function captures data uncertainty or noise. GPR provides both point predictions and predictive uncertainties, enabling robust decision-making and uncertainty quantification. The capability of GPR to handle uncertainty is particularly advantageous in the current application, where accurate predictions and confidence intervals are vital for reliable compressor performance estimation.

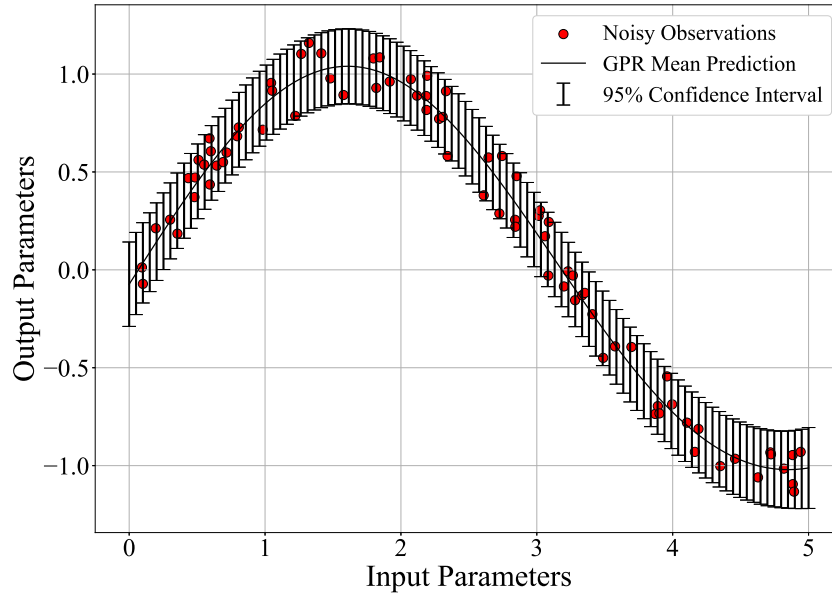


Figure 5.2: Visualisation of Gaussian Process Regression (GPR) modelling

Figure 5.2 provides an example schematic of GPR model predictions (black line) fitted to noisy data, demonstrating its ability to estimate uncertainty through the shaded 95% interval.

Given a training dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ with input vectors $\mathbf{x}_i \in R^d$ and corresponding outputs $y_i \in R$, the goal of GPR is to predict the output y_* for a new input vector $\mathbf{x}_*$. The predicted output y_* is modeled as a Gaussian distribution:

$$y_* \sim \mathcal{N}(\mu_*, \sigma_*^2) \quad (5.1)$$

The mean μ_* and variance σ_*^2 of the predictive distribution are given by:

$$\mu_* = \mathbf{k}_*^\top (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y} \quad (5.2)$$

$$\sigma_*^2 = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{k}_* \quad (5.3)$$

where $\mathbf{k}_*$ is the vector of covariances between the training data and the new input vector, $\mathbf{K}$ is the covariance matrix of the training data, σ_n^2 is the noise variance, and $\mathbf{y}$ is the vector of training outputs. The choice of covariance function (kernel) $k(\cdot, \cdot)$ plays a crucial role in GPR, allowing flexibility in capturing different data relationships.

In addition to the GPR model, several other machine learning algorithms such as Support Vector Machines (SVM), Artificial Neural Networks (ANN), and polynomial regression, were also explored to assess their performance and suitability for the given task. Briefly, these algorithms are summarised below for completeness. SVM [70], a widely used supervised learning algorithm, seeks the optimal hyperplane that best separates data points of different classes in a high-dimensional space. SVM is suitable for both classification and regression tasks and offers strong generalization capabilities. ANN [71] comprises interconnected nodes (neurons) organized in layers. It is a powerful deep learning technique capable of capturing complex relationships between input and output variables. Polynomial Regression [72] extends the traditional linear regression by fitting a polynomial function to the data. It is particularly useful when the relationship between the variables appears to be non-linear. The degree of the polynomial is a hyperparameter that can be tuned for improved model performance.

While each of these algorithms offers unique strengths and has been widely used in various domains, GPR demonstrated superior performance in terms of predictive accuracy and uncertainty quantification, making it the preferred choice for the specific compressor performance estimation task in this study.

Dataset size optimisation through initial training

The datasets generated for training machine learning (ML) models are often extensive, rendering them unsuitable for direct use in training due to the risk of overfitting or underfitting.

Overfitting occurs when the model performs exceptionally well on the training data but poorly on unseen data, while underfitting arises when the model fails to capture the underlying patterns in the training data, leading to poor performance on both training and new data instances. To address these concerns, a program was developed to determine the optimal quantity of data required for training the ML model, effectively avoiding overfitting and underfitting. The GPR model was used as the base model to assess the effect of the size of the dataset on the prediction accuracy.

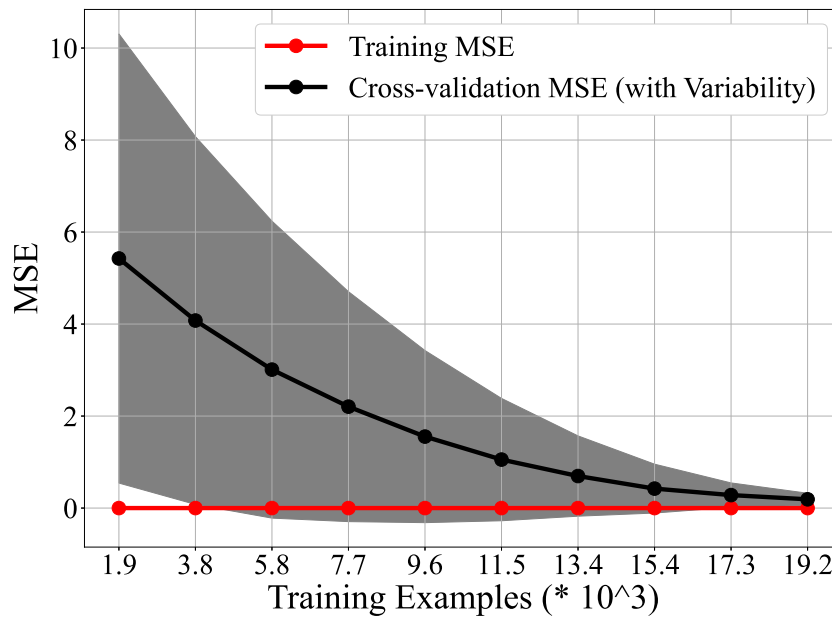


Figure 5.3: Identifying the optimal size of the dataset: Evaluation of model performance as a function of the size of the training dataset.

The model's performance was analyzed using a learning curve, as depicted in Figure 5.3. The x-axis represents the number of training examples, while the y-axis displays the mean squared error (MSE) as the performance metric. The red curve illustrates the training MSE, indicating how the model's performance improves with an increasing number of training examples. The black curve represents the cross-validation mean squared error (MSE), this plot offers insights into the model's generalization performance. As the number of training examples increases, the cross-validation MSE steadily decreases, indicating improved generalization capability. The presence of a grey shaded region complements this understanding by depicting the variance in the model's performance during cross-validation. A broader shaded region suggests higher variability across different cross-validation folds, while a narrower one signifies lower variability and greater consistency in performance. An optimal dataset size of 19200 was identified for training the model, resulting in an optimal MSE of 0.19035. This optimal MSE value reflects the model's accuracy in predicting the target variable based on the selected

features, thereby effectively capturing the underlying relationships between the input features and the target variables. Having arrived at the optimal size of the dataset, the next section will present the results of the four different ML models (including GPR), followed by the further hyperparameter tuning of the best-performing model, which in the current case was the GPR.

Model training

In this section, four machine learning (ML) models—Support Vector Machine (SVM), Artificial Neural Network (ANN), Polynomial Regression, and Gaussian Process Regression (GPR), were trained using the optimised dataset size of approximately 19,200 instances obtained from the previous section. Initially, all models were trained using default hyperparameters to establish baseline performance. Table 5.2 presents the comparative analysis of these models on both training and testing datasets.

Table 5.2: Comparison of machine learning models based on their performance on training and testing data (before tuning)

ML models	RMSE	R^2 (%)
Training result		
SVM	0.7582	53.2026
ANN	0.4984	65.1867
Polynomial	0.5259	63.8049
GPR	0.4587	67.2668
Testing result		
SVM	0.7674	40.2751
ANN	0.4979	58.3781
Polynomial	0.5439	54.3292
GPR	0.4876	64.6026

From the results, GPR emerged as the most promising model, with the lowest RMSE and highest R^2 on both datasets. However, to ensure a fair and robust comparison, all models were further subjected to hyperparameter tuning using standard optimisation strategies:

- **GPR:** Optimised using Bayesian Optimisation for the kernel length scale and noise level. Detailed in the next section.
- **SVM:** Grid search optimisation was applied to tune the kernel (RBF), regularisation parameter (C), and gamma.

- **ANN:** Hyperparameters such as the number of hidden layers, neurons per layer, activation function, and learning rate were optimised using random search with early stopping.
- **Polynomial Regression:** The polynomial degree was tuned via cross-validation, ranging from degree 2 to 5.

The performance of these models after tuning is summarised in Table 5.3, which compares their testing accuracy. The GPR model continues to outperform all other ML models post-tuning, justifying its selection as the surrogate model for screw compressor performance prediction and optimisation.

Table 5.3: Comparison of machine learning models on testing data after hyperparameter tuning

ML model	RMSE	R^2 (%)
Testing result		
GPR (Tuned)	0.010301	99.9801
ANN (Tuned)	0.061104	97.8213
Polynomial (Tuned)	0.073234	96.0279
SVM (Tuned)	0.084523	93.8465

These results confirm that GPR is not only accurate but also generalisable, which makes it particularly suitable for complex, non-linear performance mapping of screw compressors. Consequently, the next section focuses exclusively on the hyperparameter tuning strategy and internal architecture of the GPR model.

Hyperparameter tuning

Hyperparameter tuning is crucial for enhancing the predictive performance of machine learning models. In this study, Bayesian optimisation is utilized as the preferred method due to its efficiency in exploring the hyperparameter space, requiring fewer iterations than conventional techniques like grid search or random search. The kernel function's hyperparameters of the GPR model are tuned using Bayesian optimisation. The kernel comprises the Radial Basis Function (RBF) kernel and the White Kernel, with the hyperparameters to be optimised being the RBF kernel's length scales and the WhiteKernel's noise level.

Performance metrics, including Root Mean Squared Error (RMSE) and R-squared, are calculated for both training and testing datasets during the optimisation process.

The Bayesian optimisation process is mathematically described by the equation:

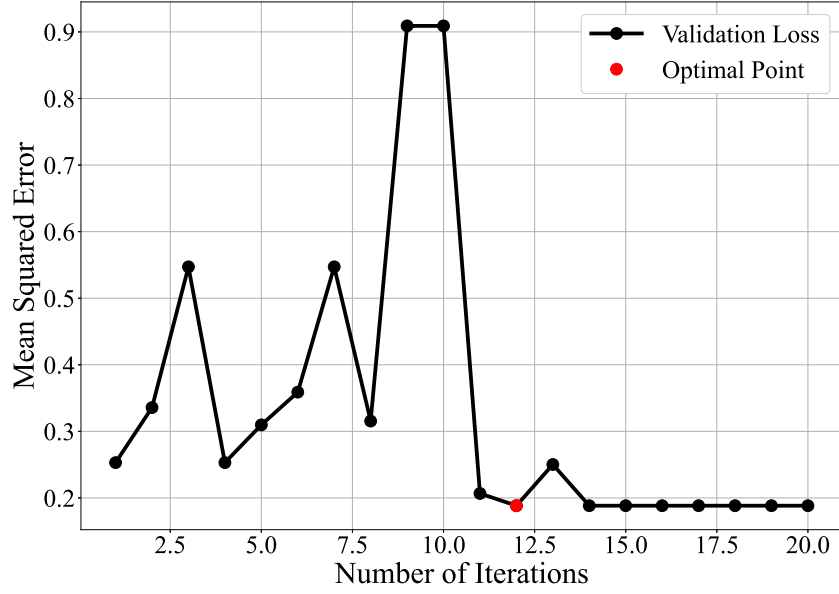


Figure 5.4: Validation loss during hyperparameter tuning of the GPR model with Bayesian optimization.

$$x_{\text{next}} = \arg \max_x \alpha(x) \cdot \mathcal{U}(x; \min, \max) \quad (5.4)$$

Where x_{next} represents the variable denoting the next point or input to be selected for evaluation in the optimisation process. It is typically a vector in the input space. $\arg \max$ symbol is used to find the argument (in this case, the value of x) that maximizes the expression following it. It means we are looking for the input x that maximizes the acquisition function $\alpha(x) \cdot \mathcal{U}(x; \min, \max)$. $\alpha(x)$ represents the acquisition function. The choice of the acquisition function depends on the specific Bayesian optimisation algorithm being used. Common choices include Expected Improvement (EI), Probability of Improvement (PI), and Upper Confidence Bound (UCB). The acquisition function quantifies the utility of evaluating the objective function at a particular input x . It guides the search by balancing exploration (trying new points) and exploitation (focusing on promising points). $\mathcal{U}(x; \min, \max)$ represents a probability distribution over the input space. In Bayesian optimisation, it is often used to model uncertainty or exploration. The notation $\mathcal{U}(x; \min, \max)$ typically denotes a uniform distribution over the input space, where $\min$ and $\max$ represent the minimum and maximum bounds for the input variables. This distribution encourages exploration within the specified bounds.

In summary, the equation describes how Bayesian optimisation selects the next input point x_{next} by maximizing the acquisition function $\alpha(x)$ while considering a probability distribution $\mathcal{U}(x; \min, \max)$ that guides the exploration of the input space. The goal is to find the input x that is expected to yield the most valuable information for optimising the objective function.

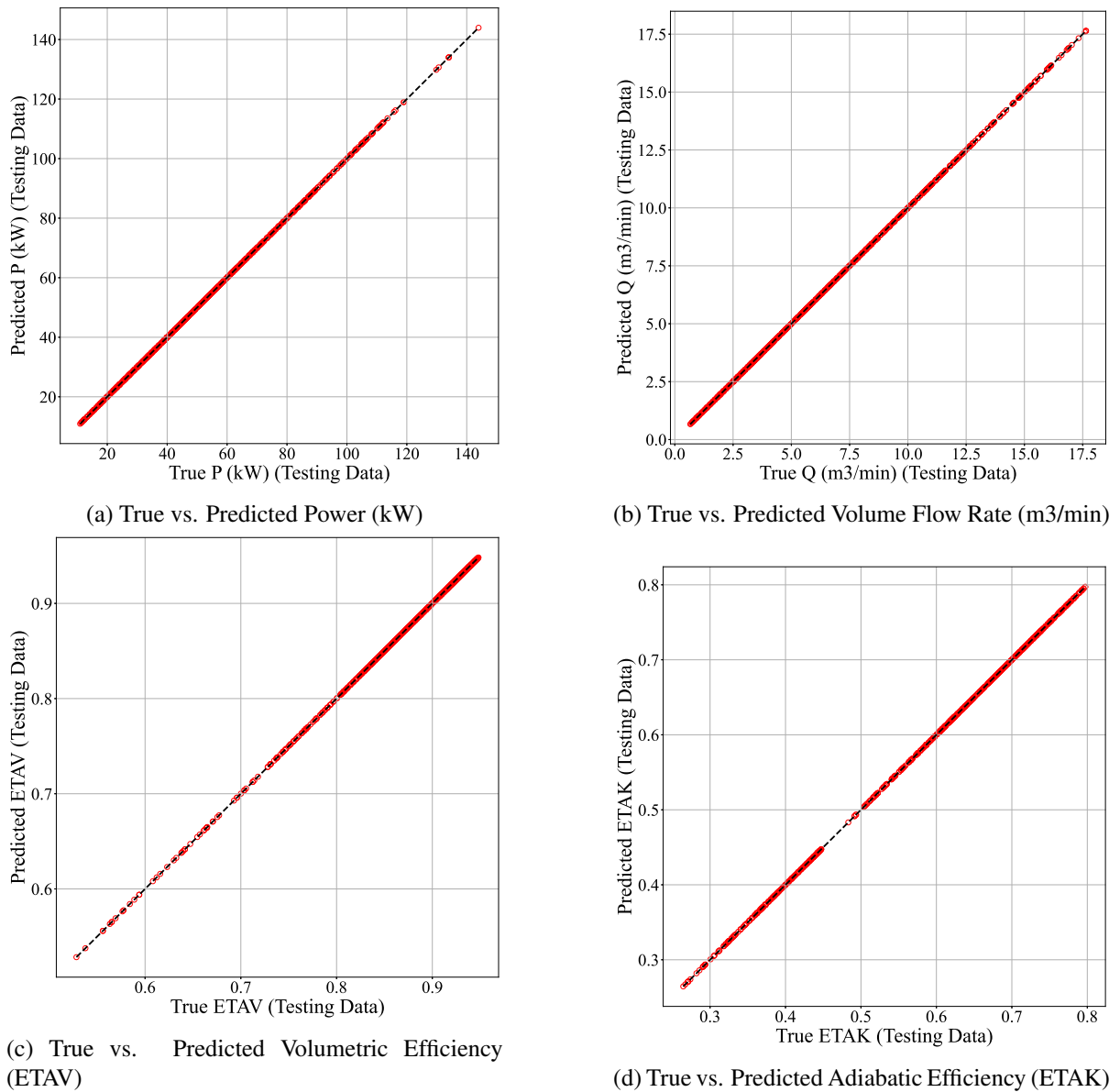


Figure 5.5: Hyperparameter-tuned GPR model predictions for the compressor performance characteristics on the test dataset: Parity plots

Figure 5.4 shows the validation loss (mean squared error) of the GPR model during hyperparameter tuning using Bayesian optimisation. The red dot represents the optimal point where the validation loss is minimized, leading to the optimal set of hyperparameters for the model. The tuned model demonstrates improved performance, evident from the substantial reduction in RMSE and the increase in R-squared values for both training and testing data. Visual comparisons of true vs. predicted values are presented in terms of parity plots in Figure 5.5.

Figure 5.6 shows the progression of training and validation loss over iterations for a GPR

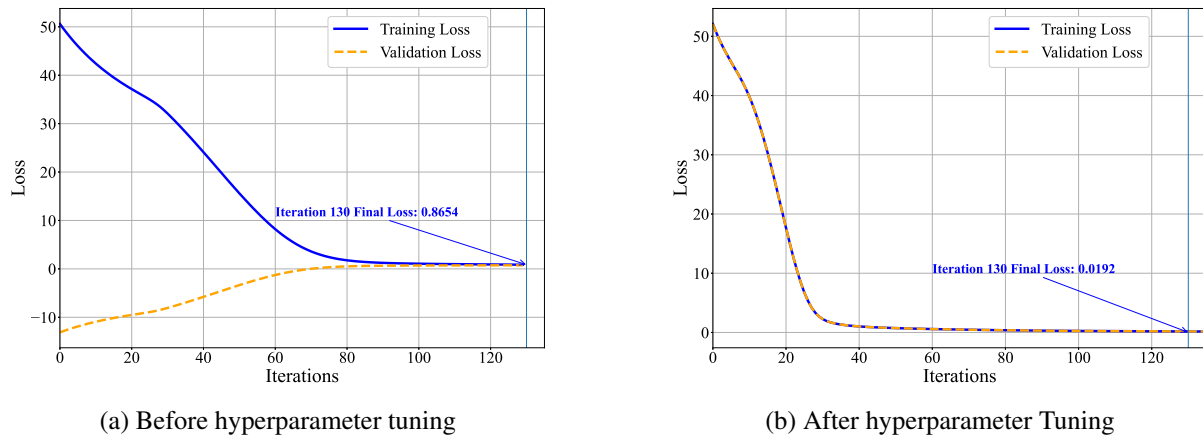


Figure 5.6: Learning curve of the GPR model before and after hyperparameter tuning

Table 5.4: Optimised hyperparameters along with their search ranges

Hyperparameter	Range	Optimal Value
Kernel Length Scale	(0.01, 10)	(8.4244, 8.8499, 7.4057, 6.3108)
Kernel Noise Level	(0.01, 100)	7.6409

model before and after hyperparameter tuning. In Figure 5.6a, the model's initial performance without hyperparameter tuning is depicted. In Figure 5.6b, the effects of hyperparameter tuning on the model's convergence are demonstrated. The dashed orange line represents validation loss, the solid blue line indicates training loss and the red dotted line marks the point of early stopping. The optimised hyperparameters are listed in Table 5.4. The GPR model's performance shows significant enhancement, thereby providing more accurate predictions (Table 5.5). This hyperparameter-tuned GPR model will be further utilized to optimise screw compressor parameters, with the ultimate goal of reducing specific power consumption.

Figures 5.7, 5.8, 5.9, 5.10 illustrate the application of Gaussian Process Regression (GPR) as a surrogate model to perform predictions of the compressor performance characteristics as

Table 5.5: Comparison of GPR performance on training and testing data before tuning and after tuning

ML model	RMSE	R^2 (%)
Training result		
GPR (before tuning)	0.458712	67.2668
GPR (after tuning)	0.010889	99.9982
Testing result		
GPR (before tuning)	0.487623	64.6026
GPR (after tuning)	0.010301	99.9801

a function of tip speed (W_{tip}), built-in volume ratio (VI), relative length (L/D) & wrap angle (ϕ). From the prediction results, it is clear that the GPR model was able to capture the complex nonlinear relationship between the output and input parameters, which can be expensive to compute through physical experiments or simulations. Importantly, the highlight of the GPR model is to quantify the uncertainty in its predictions. To demonstrate this, the GPR model is utilized to perform predictions not only in the practical range of input parameters over which it is trained but also in the out-of-distributions, called here as extraterritorial predictions.

The GPR prediction plots for various input design parameters shown in Figures 5.7, 5.8, 5.9, 5.10 comprises three key components, each providing valuable insights into the modeling and prediction process:

- **GPR Predictions (Black Star):** Represented by the black star markers, these data points signify the GPR model predictions for output parameters at various input values.
- **Chamber Model Predictions (Red Triangle):** The dotted red line serves as a ground truth and depicts the underlying true function that elucidates the intricate relationship between input and output parameters. This chamber model prediction acts as a benchmark for assessing the accuracy of the GPR surrogate model.
- **Uncertainty (Cyan):** The shaded cyan region enveloping the GPR predictions signifies the 95% confidence interval. This zone quantifies the uncertainty associated with the GPR model's predictions. It provides a crucial measure of the model's confidence in its estimates, allowing decision-makers to gauge the reliability of the results.
- **Boundary (Black Dotted Line):** The black dotted line denotes the training boundary of the GPR model. It separates two distinct regions: the territorial region on the left, where the model has been trained using observed data, and the extra-territorial region on the right, which represents uncharted territory.

Figures 5.7, 5.8, 5.9, and 5.10 collectively showcase the effectiveness of Gaussian Process Regression (GPR) in capturing complex relationships and estimating prediction uncertainties. It is interesting to note that the GPR model is accurate with unnoticeable uncertainties in its territorial range, while it clearly quantifies the uncertainties as the natural outcome in its extraterritorial predictions. From the results, it can be observed that the GPR model can predict the performance parameters (P, Q, ETAV, ETAK) as a function of rotor tip speed with very good accuracy not only in its territorial range but also in the extraterritorial or out-of-distribution

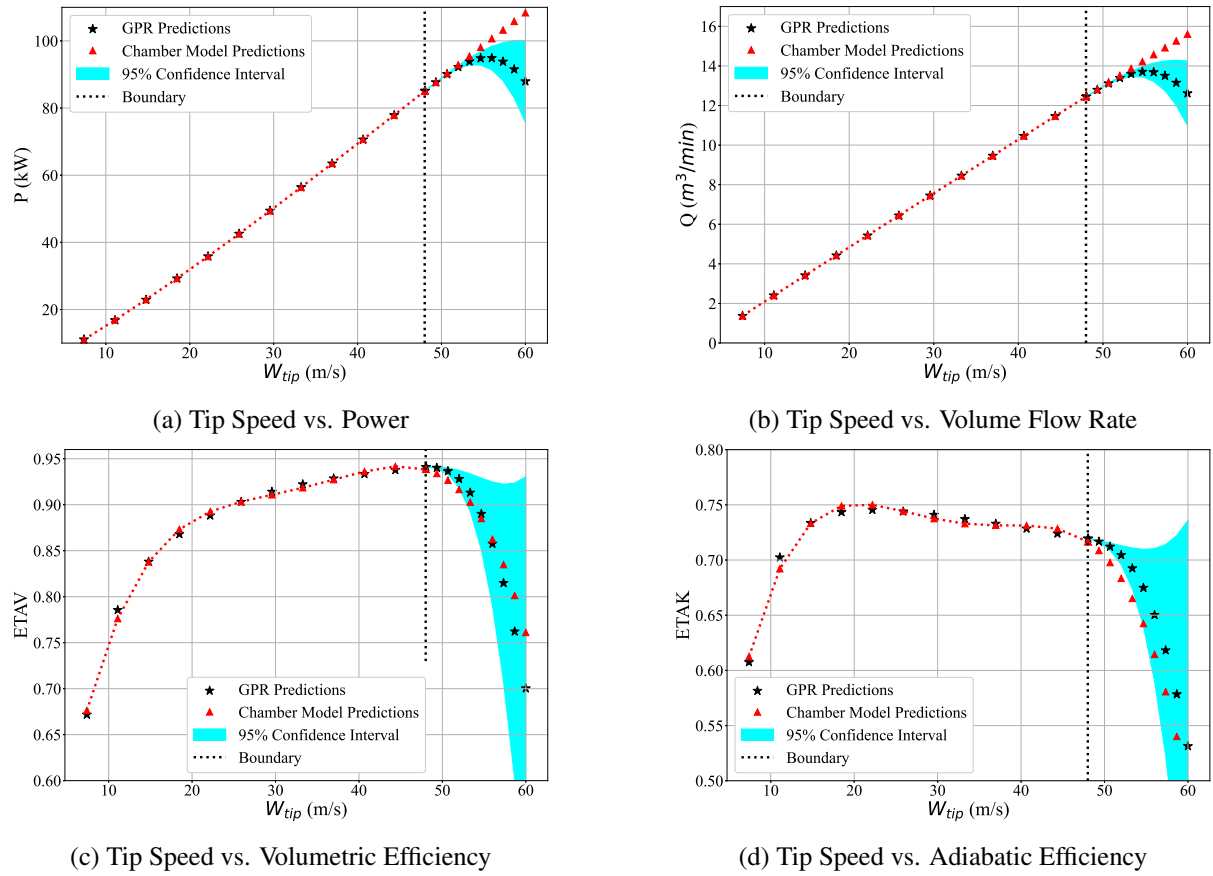


Figure 5.7: Compressor performance predictions using the GPR model for various rotor tip speeds both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

range of the input design parameters. When it comes to the other design parameters, the GPR model performs extremely well in the territorial range but deviates from physical predictions (ground truth) in the extraterritorial range, but with quantified uncertainties. It is worth emphasising here that, the territorial range considered in this study covers the entire practical range for compressor system design, making the GPR model suitable for prediction and optimisation studies. Nonetheless, using such an uncertainty-quantified surrogate model facilitates engineers and designers to make informed decisions through its quantified prediction uncertainties.

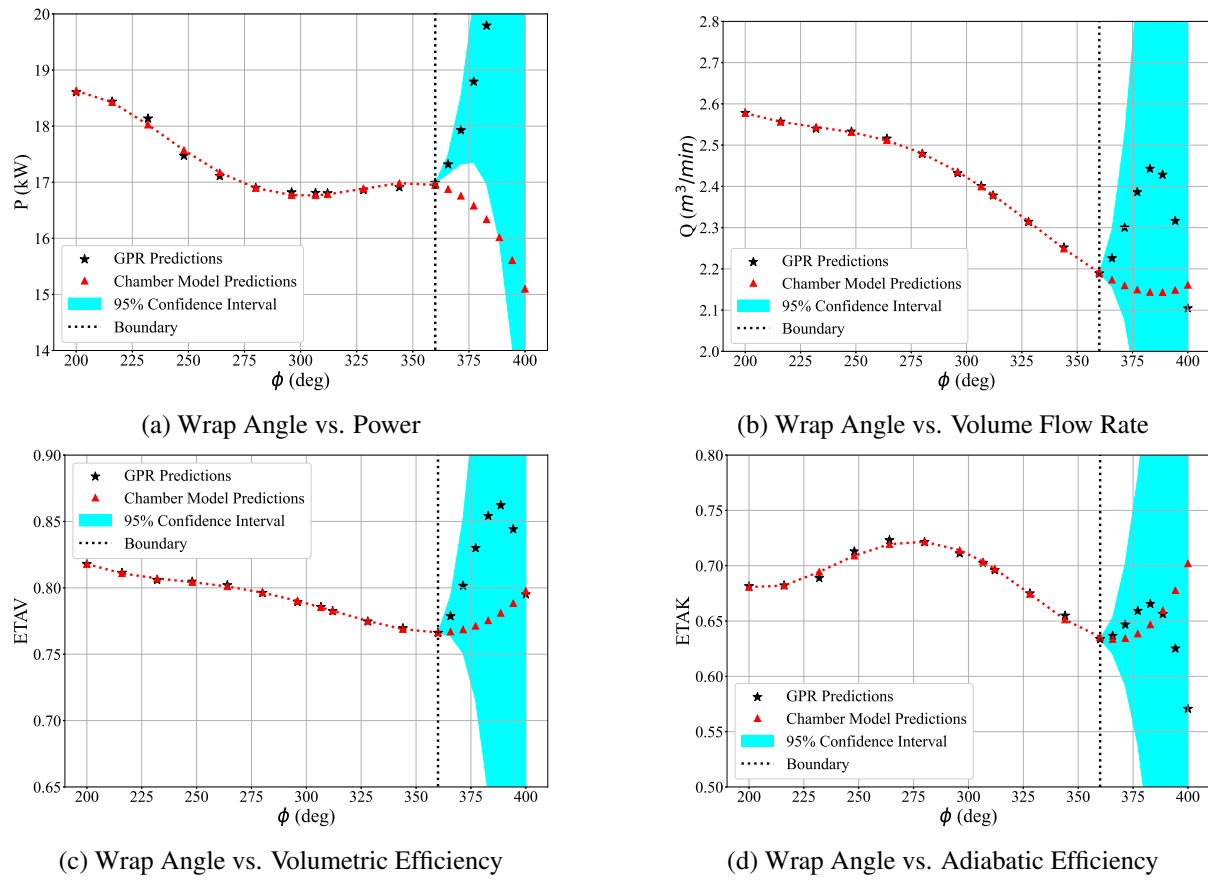


Figure 5.8: Compressor performance predictions using the GPR model for various wrap angles both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

5.2.3 Experimental validation

This section aims to verify the accuracy of the GPR based performance prediction framework within a real-world testing environment. To this end, experimental testing was conducted on the KPCL KAS-300 compressor block at the Centre for Compressor Technology, City, University of London (U.K.), employing an in-house designed air compressor test rig (Figure 5.11). This test rig adheres to the stringent CAGI and PNEUROP test standards, and testing procedures are conducted in accordance with ISO 1217 guidelines.

The test compressor, driven by a variable-speed electric motor with a rating of 75 kW, reaches a rotational tip speed of up to 40 m/s through a belt drive system with a pulley ratio of 1.7. Oil injection into the compressor occurs via a main oil supply manifold, and air enters the system through the top-mounted air intake filter. Within the compressor, the air is

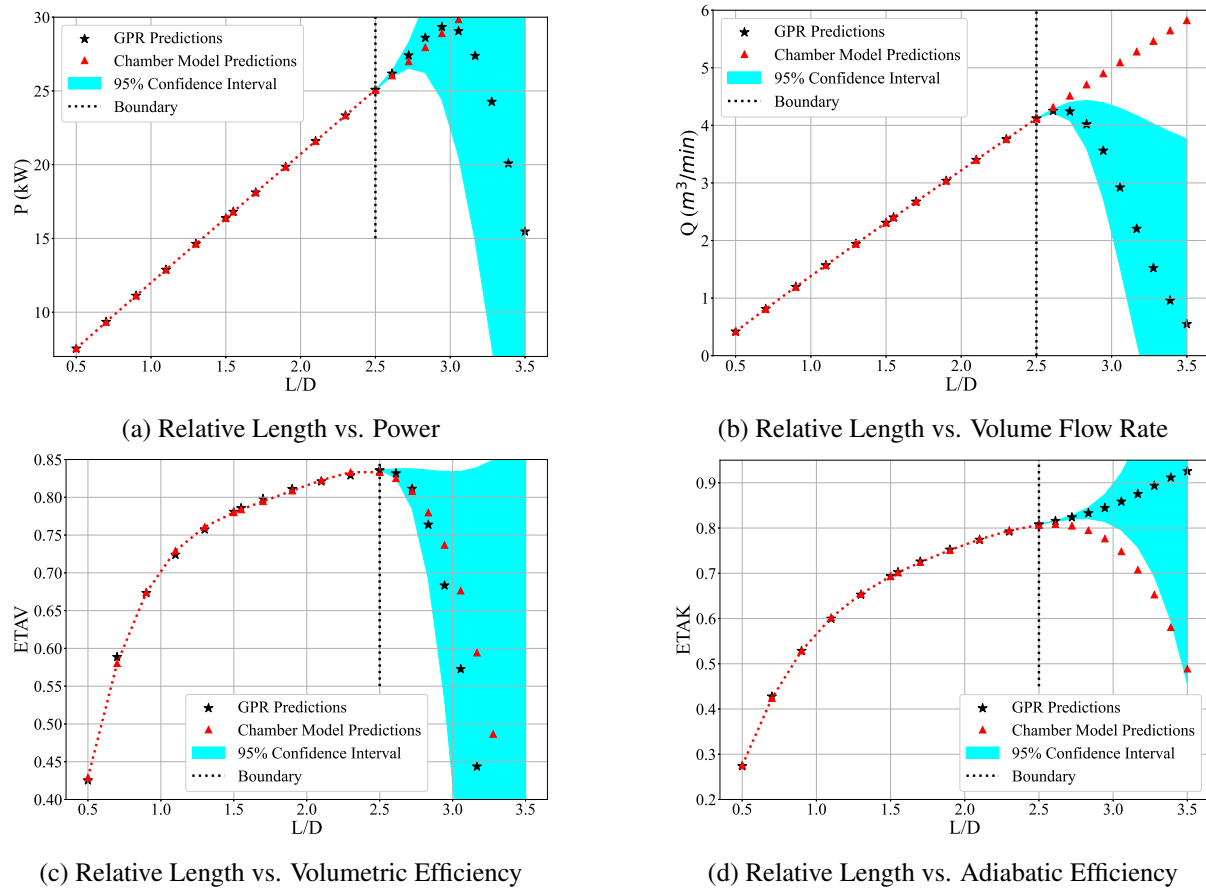


Figure 5.9: Compressor performance predictions using the GPR model for various relative rotor lengths both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

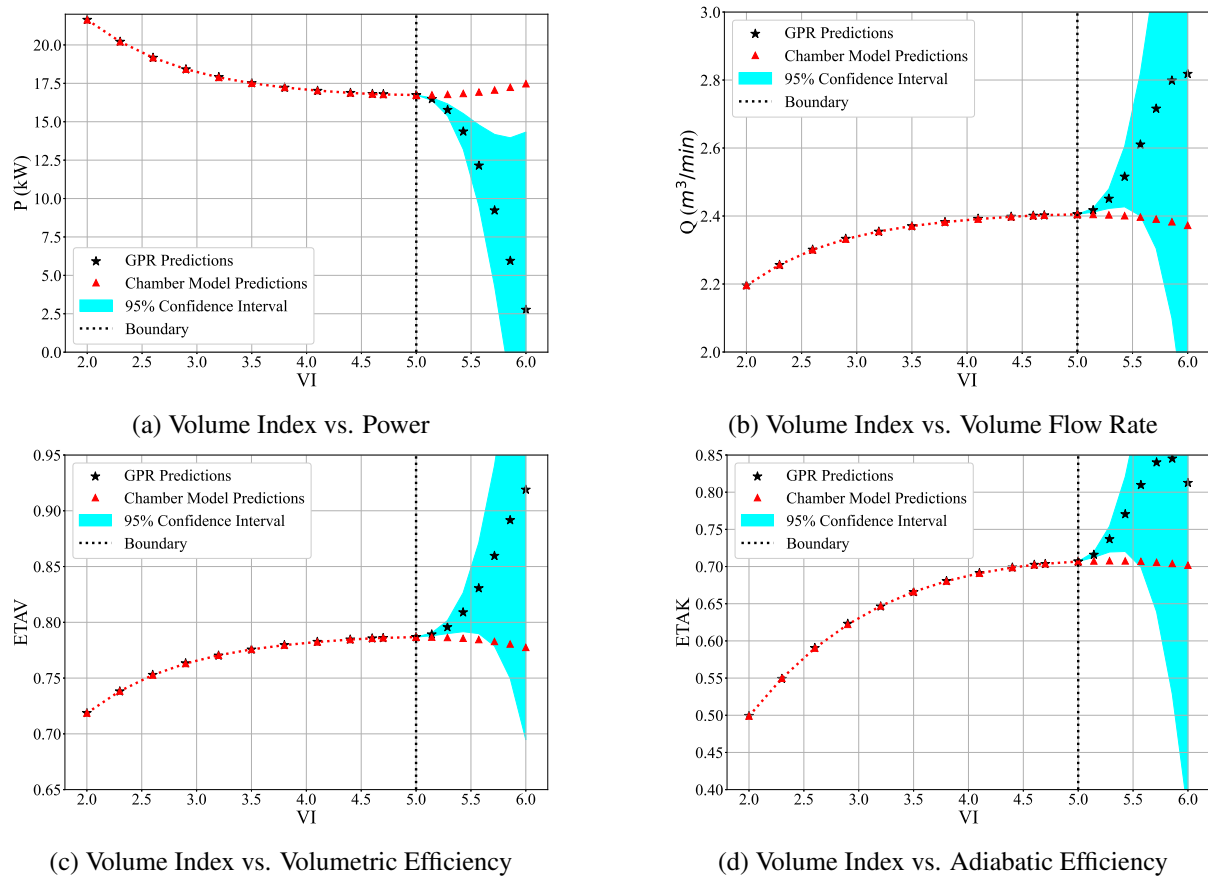


Figure 5.10: Compressor performance predictions using the GPR model for various built-in volume ratios both in territorial and extraterritorial regions along with the uncertainties. The predictions from the physics-based chamber model are plotted together for comparison.

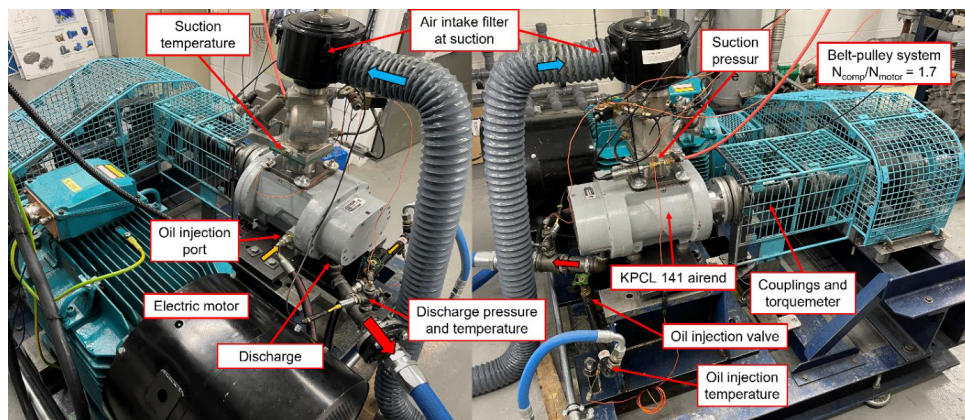


Figure 5.11: Compressor test rig showing the KAS-300 Compressor Block

mixed with oil and post-compression, the resulting mixture of hot oil and compressed air is discharged through a 2-inch pipe located at the compressor's base. Subsequently, this discharged mixture enters a two-stage oil separator system (Figure 5.12). In the first stage, a centrifugal oil separator effectively isolates the majority of the oil from the compressed air, which is then water-cooled and reintroduced into the compressor. A minor quantity of oil in vapor form proceeds to the second-stage separator, where a filter further extracts any remaining oil from the air. The collected oil in the second separator is not recirculated but is periodically filtered and reused. Finally, the air exits the system through a top-mounted pipeline equipped with an orifice plate for measuring the discharge flow rate. A globe valve, controlled by a stepper motor, offers precise regulation of discharge pressure and airflow rate, while a pressure relief valve, positioned atop the oil separator, serves as a safety precaution in the event of excess pressure buildup within the separator.

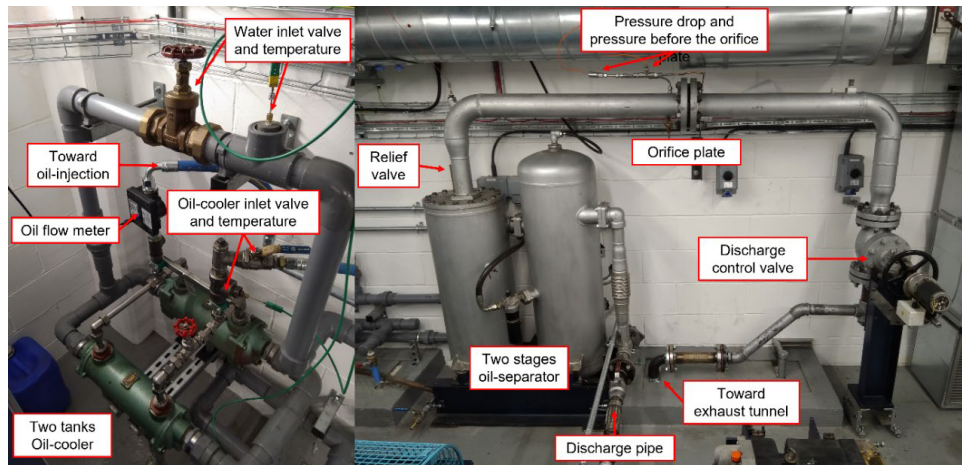


Figure 5.12: Compressor test rig - Auxiliary Systems.

In this study, the performance of the KAS-300 compressor block, operating within a pressure range of 6.5 to 14.5 bar(g) and a variable speed range of 15 to 45 m/s is investigated. The experimental analysis primarily centers on the operation of the screw compressor at a pressure ratio of 8.5. This investigation encompasses a range of tip speeds spanning from 10 to 35 m/s, while maintaining a fixed built-in volume ratio of 4.6, a relative length of 1.55, and a wrap angle of approximately 300 degrees. Throughout the experimental testing, the geometric input parameters, such as the built-in volume ratio, relative length, and rotor wrap angle, remained constant. Key performance parameters, including power consumption, volume flow rate, volumetric efficiency, and adiabatic efficiency, have been measured and are shown in Figure 5.13. Notably, since this compressor serves industrial applications, a normalised (w.r.t maximum value) performance map is presented, providing insights into its operational characteristics. The experimental data collected herein serve for the validation study, comparing the

ML model's predictions with real-world performance measurements.

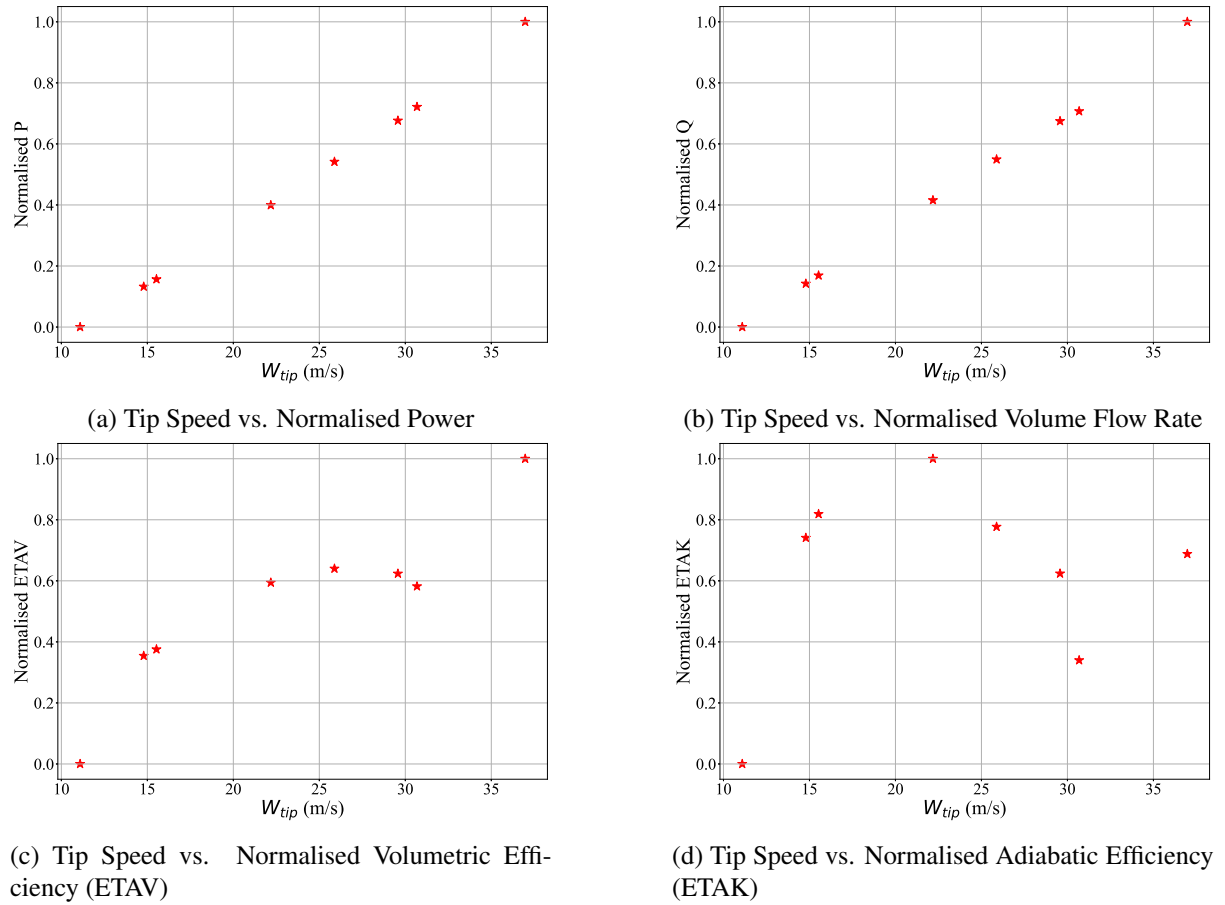


Figure 5.13: Experimental data showing the performance characteristics of the KAS-300 compressor block

The trained GPR model is then used to predict the performance of the above-specified compressor configuration for various tip speeds. The percentage error difference between the GPR model predictions and the experimental data is shown in Figure 5.14.

$$\% \text{ Error} = \frac{|\text{GPR Predictions} - \text{Experimental Data}|}{\text{Experimental Data}} \times 100 \quad (5.5)$$

The results show an overall good agreement with an acceptable deviation within the range of (+/-) 5%, validating the accuracy and reliability of the developed GPR-based performance prediction tool. The differences between the predictions and the measurements can be attributed to the testing conditions and the inherent uncertainties in the experiments.

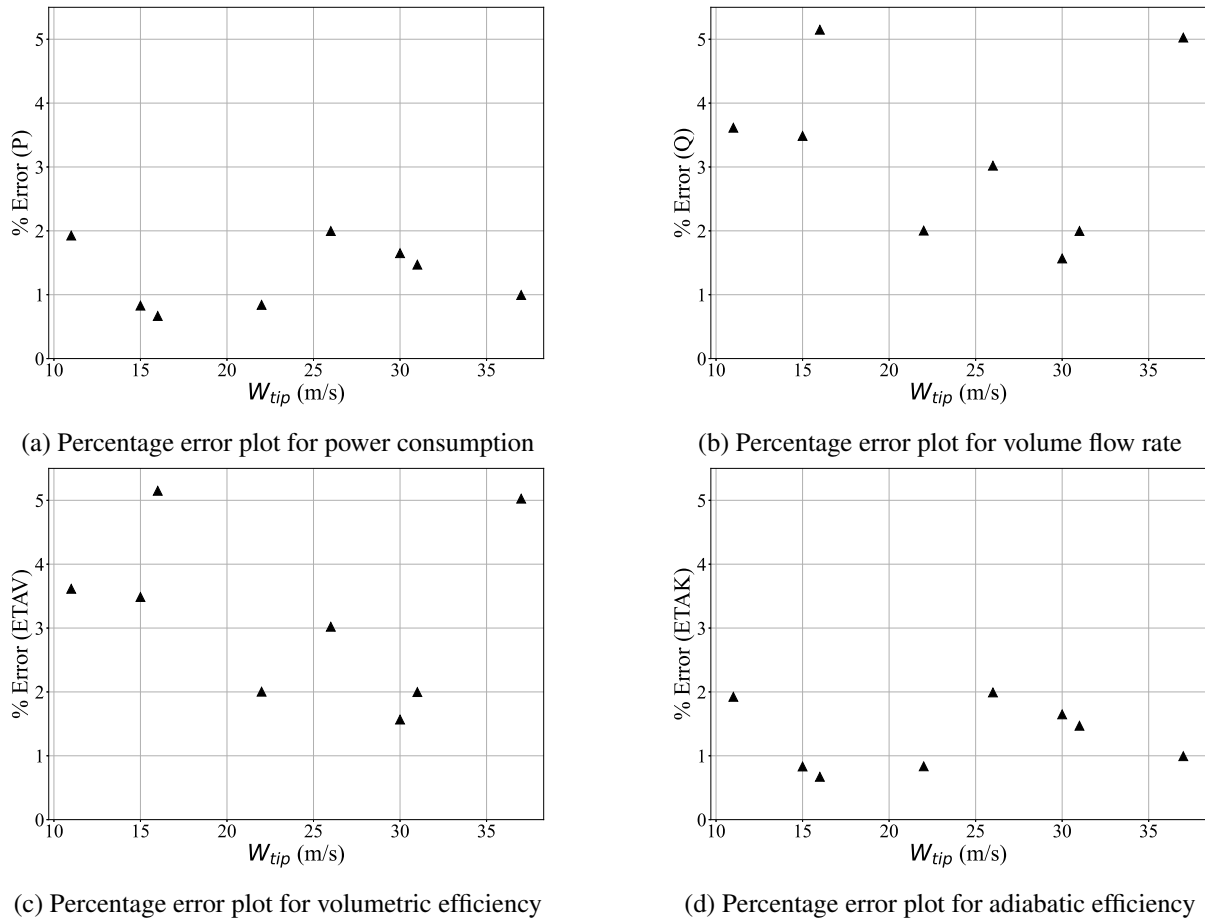


Figure 5.14: Percentage error difference between GPR predictions and experimental data for the compressor performance characteristics

5.2.4 Performance optimisation

In this section, the aim is to optimise the geometrical parameters of the screw compressor, specifically the wrap angle, relative length, tip speed of the male rotor, and built-in volume ratio. These parameters significantly impact the screw compressor's performance, with the objective of minimising power consumption and maximising the volume flow rate, volumetric and adiabatic efficiency. Bayesian optimisation is chosen for its efficient search through the parameter space, leveraging the developed Gaussian Process Regression (GPR) model. The number of iterations for Bayesian optimisation is set to 20.

The plot shown in Figure 5.15 illustrates the process of Bayesian optimisation. The y-axis represents the value of the objective function (Mean Squared Error) being minimised, while the x-axis denotes the number of iterations performed. The red marker indicates the optimal

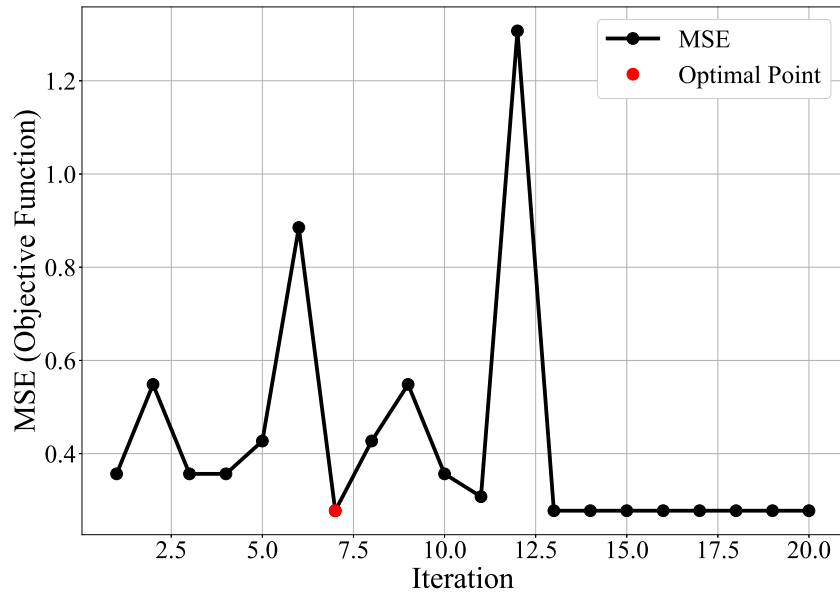


Figure 5.15: Iteration process in the Bayesian optimisation showing the loss evolution of the multi-objective function

point where the objective function reaches its minimum value, highlighting the successful convergence of the optimisation algorithm. Table 5.6 presents the input parameter range, optimal values, and optimisation duration, showcasing the effectiveness of the adopted Bayesian optimisation.

Table 5.6: Input parameters for the Bayesian optimisation and optimal values obtained

Input Parameter	Range	Optimal Value	Time Duration (min)
W_{tip} (m/s)	(15, 45)	38	29
VI	(2, 5)	4.25	29
L/D	(0.5, 2)	2	29
ϕ (deg)	(200, 360)	335.5527	29

The achieved reduction of approximately 2% in specific power consumption for the same male rotor diameter in the oil-flooded screw compressor underscores the benefits of machine learning-based optimisation.

Subsequently, the optimal geometrical parameters are validated using an alternative optimisation framework employing the Genetic Algorithm as the optimisation algorithm and the multi-chamber model as the physics solver. The evolutionary optimisation algorithm used in this study is extensively explained in [20]. Results from the multi-chamber model-based evolutionary optimisation shown in Table 5.7 align favorably with the GPR-based Bayesian opti-

misation method, further substantiating its efficacy.

Table 5.7: Input parameters for the evolutionary optimisation and optimal values obtained

Input Parameter	Range	Optimal Value	Time Duration (min)
W_{tip} (m/s)	(15, 45)	38	210
VI	(2, 5)	4.3	210
L/D	(0.5, 2)	1.99	210
ϕ (deg)	(200, 360)	330.163	210

In both optimisation frameworks, the obtained optimal values remain consistent. However, it is noteworthy that the optimisation variable 'L/D ratio' reaches its upper limit. This observation confirms the well-established notion that performance improves with an increase in rotor length. Nevertheless, it is essential to consider that the rotor length is restricted by the rotor bending deflection, which acts as a limiting factor rather than a variable for optimisation. Introducing the allowable rotor deflection as an optimisation constraint could allow us to treat the 'L/D ratio' as an optimisation variable. However, in practice, the 'L/D ratio' tends to converge to the maximum deflection limit, leaving limited room for further optimisation. Therefore, when determining the 'L/D ratio,' it is crucial to subject it to deflection analysis, which can serve as a constraint in the optimisation framework.

In summary, the current research has yielded a remarkable achievement in the development of a Gaussian Process Regression (GPR)-based machine learning algorithm for the precise prediction of screw compressor block performance. The incorporation of Bayesian optimization for hyperparameter tuning has led to a remarkable improvement in model accuracy, achieving an impressive level of nearly 99%. Furthermore, the performance prediction model underwent rigorous validation against experimental data, substantiating its reliability by demonstrating acceptable deviations within the range of (+/-) 5% in real-world scenarios.

Moreover, this work showcases the robustness of GPR models in performance predictions, primarily due to their unique ability to quantify uncertainties in predictions. The application of the hyperparameter-tuned model to optimize screw geometrical parameters through the Bayesian optimisation algorithm resulted in a notable 2% reduction in specific power consumption. Such an achievement holds profound significance within the realm of compressor design.

A comparative analysis against Genetic Algorithm (GA)-based optimization, utilizing the multi-chamber thermodynamic model, underscores the computational efficiency of the proposed framework while delivering comparable optimal values. The success of this Machine

Learning model in a single-stage context now paves the way for its generalization, intending to predict the performance for all sizes of screw compressors. Additionally, this research extends its application to multi-stage screw compressors, a forthcoming endeavor that promises innovative advancements in screw compressor technology.

5.2.5 Challenges and limitations of machine learning approach

- **Size dependency:** The accuracy of the machine learning (ML) model is highly dependent on the range of compressor sizes included in its training data. If the model is trained on a narrow range of sizes, its ability to predict performance for sizes outside this range becomes unreliable. This size dependency limits the generalizability of the model for various screw compressor configurations.
- **Data quality and availability:** The performance of ML models is only as good as the quality and variety of the training data. Incomplete, noisy, or biased data can lead to inaccurate predictions. Additionally, in the context of screw compressors, obtaining high-quality and representative datasets that capture all operating conditions can be a challenge.
- **Hyperparameter sensitivity:** The performance of the ML models is sensitive to hyperparameters, such as learning rate, regularization factors, and the number of layers or nodes in neural networks. Finding the optimal hyperparameters for a specific model can be a labor-intensive and time-consuming task. Suboptimal tuning can result in decreased prediction accuracy and subpar performance.
- **Generalization to unseen conditions:** While ML models can perform well on data similar to their training set, they often struggle to generalize to unseen operational conditions, such as extreme pressure ratios, novel compressor geometries, or different working fluids. This limits their usefulness in scenarios where out-of-sample predictions are required.
- **Model interpretability:** One of the key challenges with sophisticated ML techniques, such as deep learning and ensemble methods, is their lack of transparency. The predictions made by these models are often seen as "black boxes," making it difficult for engineers and stakeholders to interpret the results or understand the factors influencing the model's output.
- **Computational cost:** Some ML algorithms, especially those that involve complex architectures like deep neural networks or ensemble methods, can be computationally expensive to train. This becomes a limitation when dealing with real-time applications or when frequent retraining is required to accommodate new data.
- **Overfitting risk:** When the model is trained on a small dataset or a dataset that does not sufficiently represent all operational scenarios, there is a high risk of overfitting. Overfit-

ting occurs when the model learns noise in the training data, leading to poor performance on unseen data.

In conclusion, while ML-based performance prediction holds great potential for optimizing screw compressor performance, it is not without its limitations. The challenges associated with data quality, size dependency, and generalization to unseen conditions, among others, must be addressed through thoughtful model development, continuous data integration, and the application of advanced techniques for hyperparameter tuning and interpretability.

5.3 Modelling framework for multi-stage screw compressors

5.3.1 Evaluation of intermediate pressure and volume ratio

Multi-stage screw compressors are essential for high-pressure applications, as they distribute the compression process across multiple stages, improving overall efficiency and reducing excessive temperature rise. Among the most critical parameters in the design of such compressors are the intermediate pressure and the built-in volume ratio (VI). These parameters significantly impact the performance, reliability, and thermodynamic efficiency of the compressor system.

Intermediate pressure

In a multi-stage compressor, the intermediate pressure between stages plays a crucial role in distributing the work evenly across the stages. For two-stage screw compressors, the intermediate pressure P_m is calculated based on the suction pressure P_1 and discharge pressure P_2 . The general formula for intermediate pressure in a multi-stage system with z stages is given as:

$$P_m = (P_1 \cdot P_2)^{\frac{1}{z}} \quad (5.6)$$

In the case of a two-stage compression system, this expression simplifies to:

$$P_m = \sqrt{P_1 \cdot P_2} \quad (5.7)$$

This equation represents the geometric mean of the suction and discharge pressures. It ensures that the compression process is balanced between the stages, preventing excessive pres-

sure gradients that could lead to increased energy losses or overheating of the system.

As shown in the pressure-volume (PV) diagram in Figure 2.1, the intermediate pressure P_m corresponds to the point where the first stage of compression ends and the second stage begins. This intermediate pressure acts as the transition boundary, enabling the compressor to continue compression at a lower temperature due to interstage cooling. Selecting the optimal intermediate pressure not only enhances energy efficiency but also ensures reliable performance across all stages of the compressor.

Built-in volume ratio (VI)

The built-in volume ratio (VI) is another key parameter that affects the pressure ratio achieved by a screw compressor, depending on its geometric design. It is defined as the ratio of the volumes at the suction and discharge points:

$$VI = \frac{V_s}{V_d} \quad (5.8)$$

where V_s is the suction volume, and V_d is the discharge volume. The VI ratio directly influences the compressor's ability to achieve the desired compression ratio, and optimizing it ensures better thermodynamic performance. A well-designed VI ratio reduces energy consumption, improves volumetric efficiency, and minimizes temperature rise during compression.

The PV diagram (Figure 2.1) illustrates how the compression process occurs over two stages. The intermediate pressure P_m serves as the dividing point, while the built-in volume ratio controls the pressure ratio across each stage. Proper calculation of these parameters helps the compressor operate efficiently, reducing mechanical stresses and avoiding energy losses during the compression process.

Thus, the careful calculation of both the intermediate pressure and built-in volume ratio is vital for ensuring the optimal performance of multi-stage screw compressors, enhancing their operational efficiency, and prolonging their service life.

5.3.2 Boundary conditions

The selection of appropriate boundary conditions is critical for accurately modelling multi-stage screw compressors, ensuring that the system's behaviour is represented effectively. These boundary conditions encompass parameters such as inlet and outlet temperatures, mass flow rates, pressure ratios for each stage, and oil injection points, as depicted in Figure 5.16.

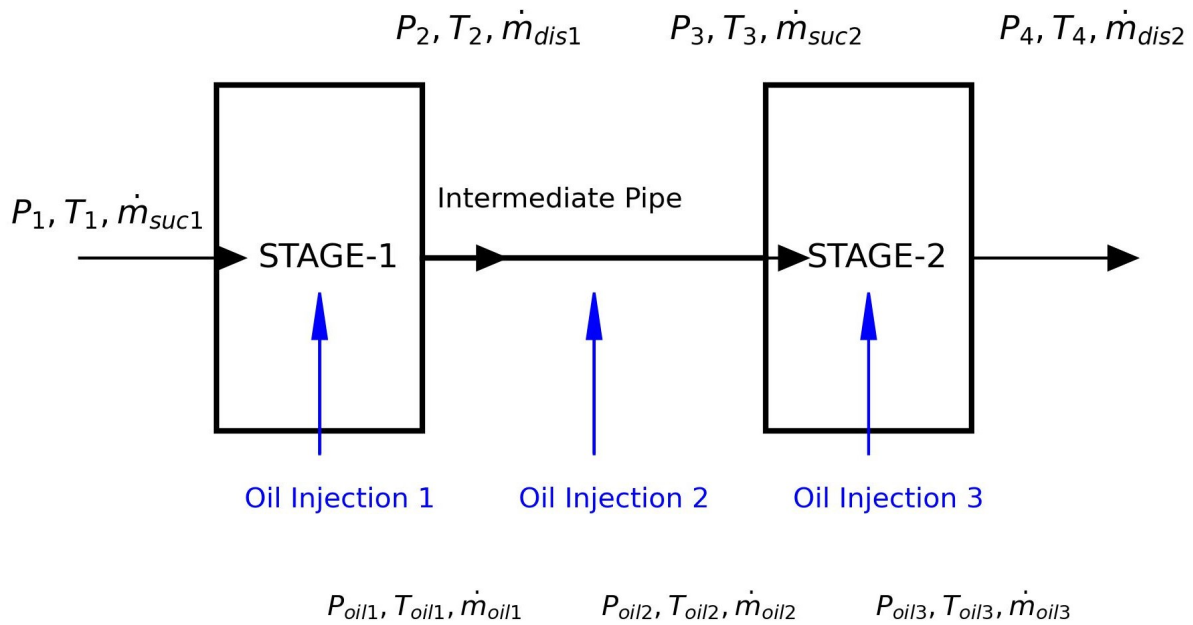


Figure 5.16: Schematic representation of a two-stage oil-injected air screw compressor.

Conservation of mass

The principle of mass conservation is key in fluid dynamics and dictates that mass cannot be created or destroyed. In the context of a two-stage screw compressor, this means the mass entering Stage 1 must equal the mass exiting Stage 2, accounting for oil mass flow rates injected into each stage:

$$\dot{m}_{suc1} = \dot{m}_{dis1} + \dot{m}_{oil1}, \quad \dot{m}_{suc2} = \dot{m}_{dis2} + \dot{m}_{oil2} \quad (5.9)$$

This ensures that the total mass flow rate remains conserved through the suction and discharge points, as illustrated in Figure 5.16.

Intermediate pressure and temperature

The intermediate pressure P_3 at the suction of Stage 2 is a critical parameter that directly impacts the efficiency and performance of the two-stage screw compressor. Typically, P_3 equals the discharge pressure of Stage 1 P_2 , but in practice, a pressure drop ΔP is often observed due to pipe friction, heat exchange, or other factors:

$$P_3 = P_2 - \Delta P \quad (5.10)$$

The interstage pressure plays a fundamental role in optimizing the total power consumption of a two-stage compressor. Ideally, it should be adjusted dynamically to minimize overall energy usage. However, in this framework, the interstage pressure has been assumed as the geometric mean of the suction and discharge pressures with a fixed pressure drop of 0.5 bar for computational feasibility. This assumption was made to ensure numerical stability in the optimization framework and to facilitate a systematic comparison of different configurations without introducing additional complexity in the optimization process.

The pressure drop ΔP between the stages is highly dependent on several factors, including the final discharge pressure, piping configuration, and fluid flow rate. At higher discharge pressures, the pressure drop tends to be larger due to the increased flow resistance in the piping system and heat dissipation. For instance, in scenarios where the final discharge pressure exceeds 21 bar, the pressure drop can reach values greater than 0.5 bar, while at lower discharge pressures (e.g., below 18 bar), the pressure drop might be less than 0.5 bar. Thus, the optimization of the intermediate pressure P_3 must account for the variability of ΔP , especially as higher discharge pressures induce more significant pressure drops. The impact of the pressure drop ΔP on the total power consumption of the compressor is illustrated in Figure 5.17. The figure demonstrates a linear increase in total power consumption with a rising pressure drop, indicating that higher pressure losses directly contribute to increased energy demand in the system.

Although fixing the interstage pressure allows the framework to operate efficiently, this simplification does not account for potential variations in power distribution between the LP and HP stages, which could lead to a suboptimal overall power consumption. Previous industrial studies [50] have demonstrated that adjusting the interstage pressure dynamically—rather than assuming it as a geometric mean—can lead to significant reductions in specific power, as the most energy-efficient operating point does not always align with the theoretical geometric

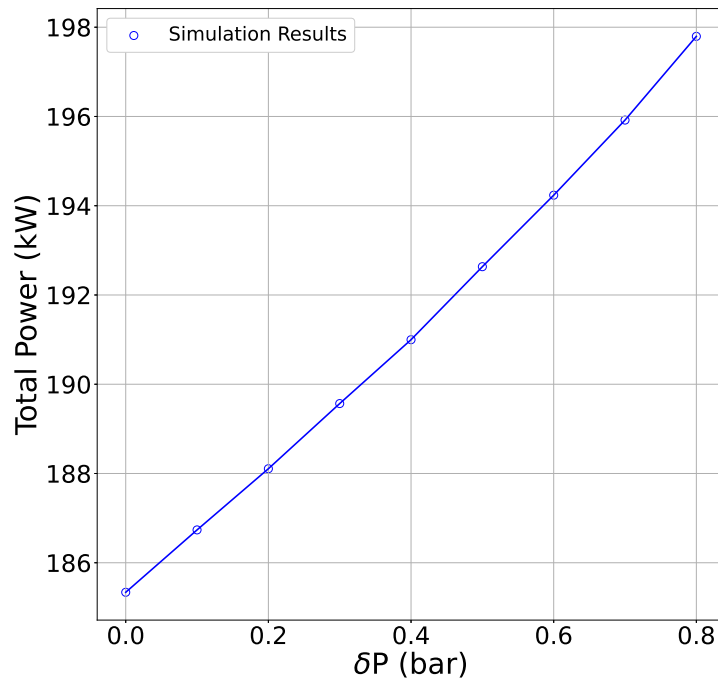


Figure 5.17: Variation of total power with pressure drop for a two-stage screw compressor having a discharge pressure of 23 bar.

mean.

In this research, the SCORG software was used to generate the optimization dataset, and since SCORG already incorporates suction and discharge pressure losses in the performance calculations, additional pressure losses were not manually added. Furthermore, since the gear-driven bull-gear arrangement in the two-stage compressor imposes constraints on speed ratios between LP and HP rotors, the variation of interstage pressure would also affect the shaft power balance, necessitating a more complex optimization approach.

While the current framework does not optimize interstage pressure, this remains an important future research direction. A fully optimized model would include interstage pressure as a variable in the multi-objective optimization process, allowing the system to iteratively adjust P_3 based on total power minimization rather than a fixed geometric mean assumption. This aspect could be explored further by implementing independent-drive two-stage compressors, where interstage pressure can be actively controlled to minimize energy consumption dynamically.

Intermediate temperature considerations

Similarly, the intermediate temperature T_3 at the suction of Stage 2 is typically equal to the discharge temperature T_2 of Stage 1, but a temperature drop ΔT may occur due to cooling losses:

$$T_3 = T_2 - \Delta T \quad (5.11)$$

Both the pressure drop ΔP and temperature drop ΔT need to be considered during the optimization process to minimize energy losses and ensure efficient compression between stages. Therefore, the optimization of intermediate pressure P_3 , accounting for variations in ΔP , remains a key area for future research to enhance performance and energy efficiency further.

In summary, the current framework assumes a geometric mean interstage pressure for computational simplicity, but a more refined model should integrate interstage pressure as an optimization variable, particularly in applications where independent control of interstage parameters is feasible. Future work should focus on implementing dynamic interstage pressure optimization strategies to achieve the lowest total power consumption, considering varying discharge pressures and operating conditions.

Oil injection and its impact

In addition to the mass flow of the working fluid, oil is injected at different points to provide cooling and lubrication. The oil injections $\dot{m}_{oil1}, \dot{m}_{oil2}, \dot{m}_{oil3}$ need to be accounted for in both mass conservation and the thermodynamic modelling of the compressor, as they influence both cooling efficiency and the overall mass balance.

Summary of boundary conditions

The boundary conditions for a two-stage screw compressor are centred on the following:

- Conservation of mass for each stage, ensuring the mass entering and exiting is balanced.
- Intermediate pressure and temperature adjustments that account for the losses occurring between stages.

- Oil injection at various points, contributing to both the mass balance and the thermodynamic efficiency of the system.

These boundary conditions are essential for accurate modelling, optimization, and design of multi-stage screw compressors, ensuring that the system operates effectively and efficiently.

5.3.3 Physical assumptions in modelling framework

The development of the multi-stage screw compressor modelling framework necessitated a set of simplifying assumptions to manage computational complexity and enable scalable optimisation. These assumptions are justified based on thermodynamic reasoning, experimental insights, and constraints imposed by the simulation environment.

1. Intermediate pressure assumption

The intermediate pressure P_{int} between the stages is estimated using the geometric mean of the suction and discharge pressures, with a small pressure loss offset:

$$P_{\text{int}} = \sqrt{P_{\text{in}} \cdot P_{\text{out}}} - 0.5 \text{ bar} \quad (5.12)$$

This offset of 0.5 bar accounts for the typical pressure losses encountered in the inter-stage piping and valves. By fixing P_{int} , the optimisation space is significantly reduced, avoiding the complexity of treating it as a design variable.

2. Built-in volume ratio (VI) calculation

The built-in volume ratio (VI) for each stage is estimated using the ideal gas law and the isentropic relation between pressure and volume for an ideal gas:

$$\text{VI} = \left(\frac{P_{\text{dis}}}{P_{\text{su}}} \right)^{\frac{1}{k}} \quad (5.13)$$

where P_{dis} and P_{su} are the discharge and suction pressures of the stage, respectively, and

k is the isentropic index (typically $k = 1.4$ for air). This approach simplifies the model logic while maintaining thermodynamic accuracy.

3. Intermediate temperature assumption

The intermediate temperature T_{int} , which serves as the suction temperature for the second stage, is assumed based on the discharge temperature of the first stage minus an experimentally justified cooling offset:

$$T_{\text{int}} = T_{\text{dis},1} - \Delta T_{\text{cooling}} \quad (5.14)$$

The cooling offset $\Delta T_{\text{cooling}}$ is assumed to be 20°C , based on experimental observations and thermal analysis of the inter-stage piping. The heat loss is a combination of convective cooling and oil injection. The assumption is validated using a first-principles energy balance:

$$Q = h \cdot A \cdot (T_{\text{dis},1} - T_{\text{ambient}}) \quad (5.15)$$

$$m \cdot c_p \cdot \Delta T = Q \quad (5.16)$$

where:

- h = convective heat transfer coefficient ($\approx 30 \text{ W/m}^2 \cdot \text{K}$),
- A = surface area of inter-stage pipe ($\approx 0.05 \text{ m}^2$),
- m = mass flow rate of air ($\approx 0.1 \text{ kg/s}$),
- c_p = specific heat capacity ($\approx 1005 \text{ J/kg} \cdot \text{K}$).

Using these values, the calculated ΔT lies in the range of $(18 \sim 22)^\circ\text{C}$, supporting the 20°C assumption.

4. Mass flow balancing via speed optimisation

To ensure mass continuity between the two stages, the speed of the second stage is treated as an optimisation variable. The goal is to maintain:

$$\dot{m}_1 = \dot{m}_2 \quad (5.17)$$

This balance avoids accumulation or starvation of mass between the stages and ensures that the multi-stage model operates under steady-state flow conditions. By adjusting the rotational speed of the second stage accordingly, mass flow equilibrium is preserved.

5.3.4 Model architecture

The modelling framework developed for multi-stage screw compressors is structured to allow for flexibility in control variables, optimization parameters, and performance metrics. This architecture facilitates both single and multi-objective optimization tailored to specific application needs.

Control variables and optimisation parameters

The input parameters for the model are defined based on the application and type of optimization desired. These control variables include:

- **Input parameters:** These parameters define the operating conditions of the screw compressor and are crucial for setting up the initial boundary conditions for the system.
 - **P_{suc} in bar:** Suction pressure — This is the pressure at the inlet of the compressor and directly influences the compressor's capacity and performance.
 - **P_{dis} in bar:** Final discharge pressure — The pressure at the outlet of the compressor. Higher discharge pressures require greater energy input and affect compressor efficiency.
 - **T_{suc} in K:** Suction temperature — The temperature of the fluid entering the compressor. A lower suction temperature can improve compression efficiency by reducing the energy needed for the process.

- **N in RPM:** Speed of the male rotor — The rotational speed of the male rotor, which directly affects the volumetric flow rate and power consumption of the compressor.
- **Working fluid:** Air or other gases — The type of fluid being compressed (e.g., air, refrigerant, or other gases). Different fluids have varying properties like viscosity and thermal conductivity, which impact performance.
- **Profile clearances:** Clearances between the male and female rotor profiles significantly impact performance. Larger clearances tend to increase leakage and reduce volumetric efficiency. Optimizing the clearances is crucial for minimizing energy losses.
 - **GAPI in μm :** Interlobe clearance between the male and female rotors.
 - **GAPR in μm :** Radial clearance affecting rotor-to-housing interaction.
 - **GAPA in μm :** Axial clearance between the rotor tips and the housing.
- **Design parameters:** Wrap angle, rotor length/diameter ratio, and built-in volume ratio (VI) are crucial for determining the performance of the compressor. These parameters define the screw rotors' profiles and directly influence efficiency and compression capability.
 - **L/D:** Length-to-diameter ratio, an important geometric factor influencing rotor design.
 - **ϕ in rad:** The wrap angle, which affects the amount of compression per rotor turn.
 - **VI:** Built-in volume ratio, determining the pressure ratio of the compressor.
- **Fluid injection parameters:** Fluid parameters such as oil viscosity, pressure, and temperature are critical in influencing heat transfer and minimizing temperature rise across stages. Optimizing fluid injection parameters ensures enhanced cooling and lubrication, contributing to compressor efficiency.
 - **P_{oil} in bar:** The oil injection pressure, which impacts the cooling and lubrication efficiency.
 - **T_{oil} in K:** Oil temperature, important for assessing the heat dissipation during compression.
 - **θ in rad:** The angle of oil injection relative to the rotor position.
 - **D_{oil} in mm:** Diameter of the oil injection nozzle, affecting flow rates and distribution.

Once the input parameters are set, the model allows users to select specific optimization targets, depending on the focus of the application. The available optimization paths include:

- **Profile clearance optimization:** Optimizing the clearances between the rotors is crucial for maximizing efficiency. Larger clearances (GAPI, GAPR, GAPA) typically result in performance deterioration due to increased leakage. Reducing the clearances to an optimal level improves volumetric efficiency and minimizes energy losses.
- **Design optimization:** Focusing on mechanical design parameters such as wrap angle, relative length, and built-in volume ratio, this optimization improves the overall reliability, thermal performance, and longevity of the compressor. Adjusting rotor geometry, for instance, can help reduce mechanical stress while improving compression efficiency.
- **Fluid injection optimization:** By optimizing fluid parameters like oil pressure, injection angles, and temperature, the system ensures effective heat transfer, minimized pressure drops, and enhanced performance across stages. In multi-stage systems, this can significantly improve the thermodynamic efficiency and reduce energy consumption.

These control variables and optimization paths allow the model to be highly versatile, enabling users to fine-tune the screw compressor's performance based on application requirements. The ability to optimize multiple parameters in both single and multi-objective frameworks ensures that the system operates efficiently, reliably, and with the desired performance metrics (refer Appendix B).

Flowchart of model architecture

The model design centres on the interaction between control variables and performance measures, providing a definitive framework for establishing optimisation objectives, whether singular or multiple. The model initiates using input parameters, including flow, power, and pressure ratio. These characteristics correspond to several stages of the compressor, after which certain optimisation objectives can be identified. The performance indicators offer insights for system assessment and subsequent design enhancement.

Figure 5.18 depicts the progression of input parameters via the model architecture. The process commences with fundamental input variables (flow, power, and pressure ratio) and advances through a mapping of the stage count. Users thereafter specify rotor profile clearances,

geometrical characteristics, and fluid injection qualities, all of which may be optimised according to application requirements. Upon completion of the stage interactions, the physics solver is executed utilising techniques such as the chamber model or machine learning-based Gaussian Process Regression (GPR) [9, 50].

This approach enables users to effectively optimise the design of the multi-stage screw compressor for diverse aims, yielding critical performance measures such as power consumption, volumetric efficiency, and specific power consumption. The model's adaptability allows for modifications according to rotor clearances, design specifications, and fluid injection parameters.

The screw compressor framework's model architecture offers users a robust tool for optimising compressor design across various parameters. The user may pick control variables pertaining to geometry, design, and fluid dynamics, subsequently choosing optimisation pathways that yield performance measurements to enhance the design for either single or multi-objective objectives.

5.3.5 Graphical user interface

The constructed Graphical User Interface (GUI), illustrated in Figure 5.19, enables users to engage effortlessly with the modelling framework of the screw compressor design and optimisation tool. The interface is engineered for simplicity and efficacy, offering a complete array of input fields and controls for optimisation activities.

The tool incorporates two solver options:

- **Chamber Model:** This solver utilises a physics-based model that considers the thermodynamics of the chamber throughout the compression process [9].
- **Gaussian Process Regression (GPR):** A machine learning solver utilising Gaussian Process Regression to forecast performance from historical data and statistical inference, offering an alternative to conventional models [50].

The interface is crafted to enhance the user experience, allowing both novice and experienced users to efficiently simulate and optimise compressor designs.

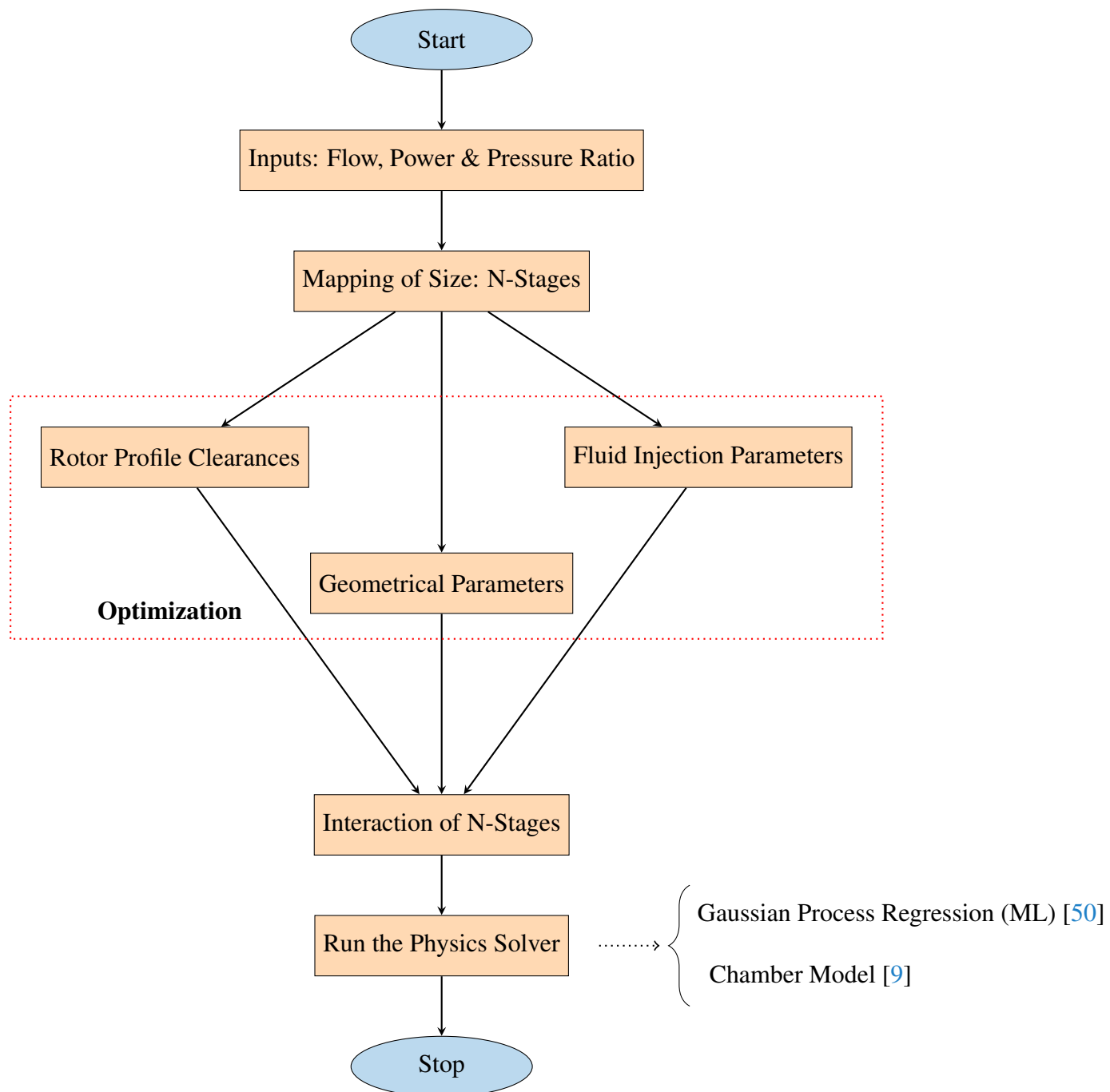


Figure 5.18: Flowchart depicting the model architecture for multi-stage screw compressor design, showing the progression of inputs, mapping, optimization, and physics solver stages.

MATLAB App

MODELLING FRAMEWORK: KIRLOSKAR PNEUMATIC CO. LTD.

Compressor Size Prediction | Single-Stage Optimisation | Multi-Stage Optimisation

INPUT

Suction Pressure (bar) Discharge Pressure (bar)

Suction Temperature (K) Male Rotor Speed (RPM)

OPTIMISATION FUNCTION

L/D Φ (rad)

VI

OPTIMISATION METHOD

Lower Limit

Upper Limit

OUTPUT FUNCTION

ETAV Power

ETAK Flow

SOLVER

Chamber Model

Figure 5.19: Graphical User Interface of the modelling framework.

5.3.6 Experimental validation

A prototype of a two-stage air screw compressor was conceived and manufactured for water-well applications to assess the theoretical outcomes and lifetime cost analysis outlined in this study. The compressor was designed to function within a power range of 290 to 308 kW, producing discharge pressures from 21 to 25 bar. The low-pressure (LP) stage functions at 3000 RPM, and the high-pressure (HP) stage operates at 3700 RPM, delivering a flow rate of roughly 1150 cubic feet per minute (CFM). The low-pressure (LP) stage features a 4/6 lobe configuration, while the high-pressure (HP) stage adopts a 6/8 lobe design, optimising efficiency and ensuring smoother operation throughout the compression process. The choice of a 6/8 lobe combination in the second stage is driven by its ability to withstand higher pressures while minimizing rotor deflection. A higher lobe count enhances rotor rigidity, reducing mechanical stresses and ensuring reliable operation under elevated pressure conditions. Additionally, the increased number of lobes improves sealing effectiveness, reducing internal leakage and enhancing overall volumetric efficiency at high-pressure ratios. The two-stage compressor is driven by a single engine shaft, which is connected to a bull gear that powers the compressor block. The LP and HP stages are each driven by pinion gears mounted on their respective main

rotor shafts. The gear arrangement of the two-stage screw compressor system is illustrated in Figure 5.20, providing insights into the drivetrain configuration, including the bull gear and pinions that drive the low-pressure (LP) and high-pressure (HP) rotors. Additionally, an isometric view of the 3D model of the compressor block is included in the same figure, showcasing the overall design before manufacturing. After fabrication, the bare two-stage screw compressor is presented in Figure 5.21, offering a visual representation of the final prototype. Due to proprietary restrictions, further technical specifications regarding the compressor design cannot be disclosed.

The experimental apparatus was carefully designed to comply with the ISO 1217 standard for displacement compressor evaluation, guaranteeing precise and consistent outcomes. The experimental setup is depicted in Figure 5.22. The prototype underwent a series of performance evaluations under steady-state settings, with the compressor functioning at specified operating points until stable parameters, including pressures, temperatures, and rotating speeds, were attained. Data gathering initiated solely after the system attained thermal and mechanical equilibrium, hence guaranteeing dependable performance data.

Each test was executed for a minimum of 10 minutes to obtain reliable performance measurements. Data was collected at intervals and averaged across several samples to reduce transitory fluctuations, and the data were normalised to the specified pressure ratios and rotor speeds for comparison. The processes were meticulously executed to guarantee that the test findings conformed to industry standards, yielding dependable performance benchmarks for subsequent study.

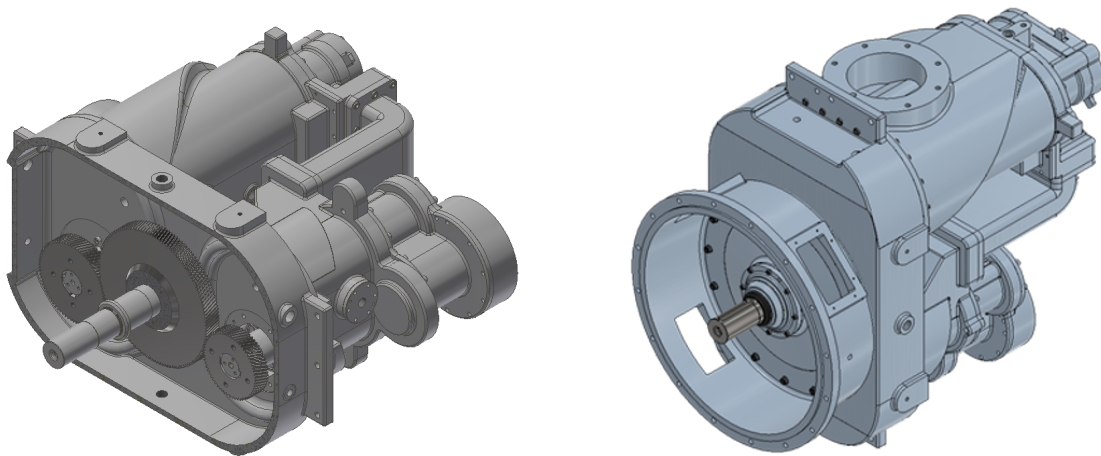
Test setup requirements:

1. **Inlet temperature:** Normal: 40°C, Highest: 50°C, Lowest: 0°C
2. **Discharge temperature:** Normal: 90-95°C, Shutdown: 105°C (manual by-pass)
3. **Oil temperature:** Normal: 62°C, Highest: 70°C
4. **Oil type:** Mineral oil (ISO VG 68)
5. **Unloading condition:** Capacity is regulated down to zero via inlet valve throttling
6. **Regulating pressure range:** Discharge pressure (P_d) $\pm 5\%$

Compressor operating conditions:

1. **Bearing life:** 18,000 hours (L10h) @ 1200 CFM / 23.41 bar (a); 15,000 hours (L10h) @ 1200 CFM / 25.13 bar (a)
2. **Seal life:** 2 years or 10,000 - 12,000 hours
3. **Pressure test:** $350 \text{ psig} * 1.1 * 1.5 = 557 \text{ psig}$ (38.41 bar g / 39.41 bar a)
4. **Operating speed:** 1470 RPM (Electrical) / 1500 - 1900 RPM (Engine), with two different gear ratios

The performance test findings are encapsulated in Table 5.8, emphasising critical parameters including power consumption, rotational speeds, interstage pressure, and compressor capacity under both testing situations.



(a) Gear arrangement with a bull gear (129 teeth) and pinions (81 and 61 teeth) on the LP and HP rotor shafts.

(b) Isometric view of the 3D model of the two-stage oil-flooded air screw compressor block.

Figure 5.20: Illustration of the two-stage screw compressor: (a) gear arrangement and (b) isometric view of the 3D model of the compressor block.

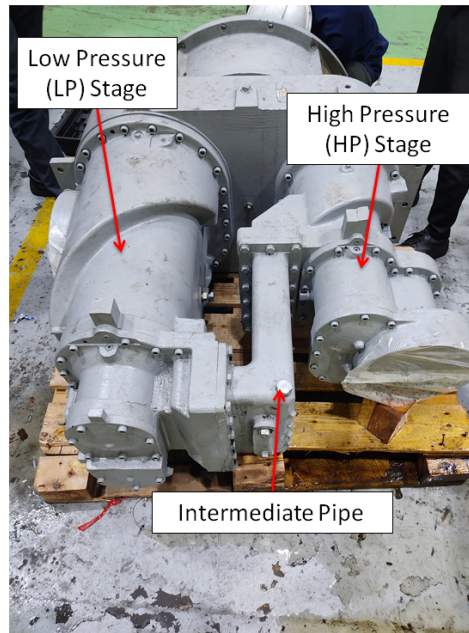


Figure 5.21: Post-manufacturing schematic of the two-stage oil-flooded air screw compressor block.

Table 5.8: Performance testing results of the two-stage air screw compressor.

Parameters	Testing-1	Testing-2	Testing-3
Inlet Suction Pressure (bar a)	0.95	0.95	0.95
Interstage Pressure (bar a)	5.07	5.20	5.37
Discharge Pressure (bar a)	21.54	23.31	25.07
Power, LP (kW)	143.18	143.18	143.18
Power, HP (kW)	146.91	155.11	164.06
Total Power (kW)	290.09	298.29	307.24
Engine RPM	1900	1900	1900
LP, RPM	3026	3026	3026
HP, RPM	3713	3713	3713
Capacity (m^3/min)	32.59	32.56	32.56

5.3.7 Chamber model predictions for two-stage screw compressors

The chamber model developed in this research serves as a digital representation of a two-stage screw compressor, enabling the generation of synthetic data for comprehensive performance analysis. The primary objective of this model is to create a reliable dataset that can be utilized to train and validate machine learning-based predictive tools. By accurately simulating compressor behavior across varying operating conditions, this digital framework provides an efficient means for performance optimization and design evaluation.

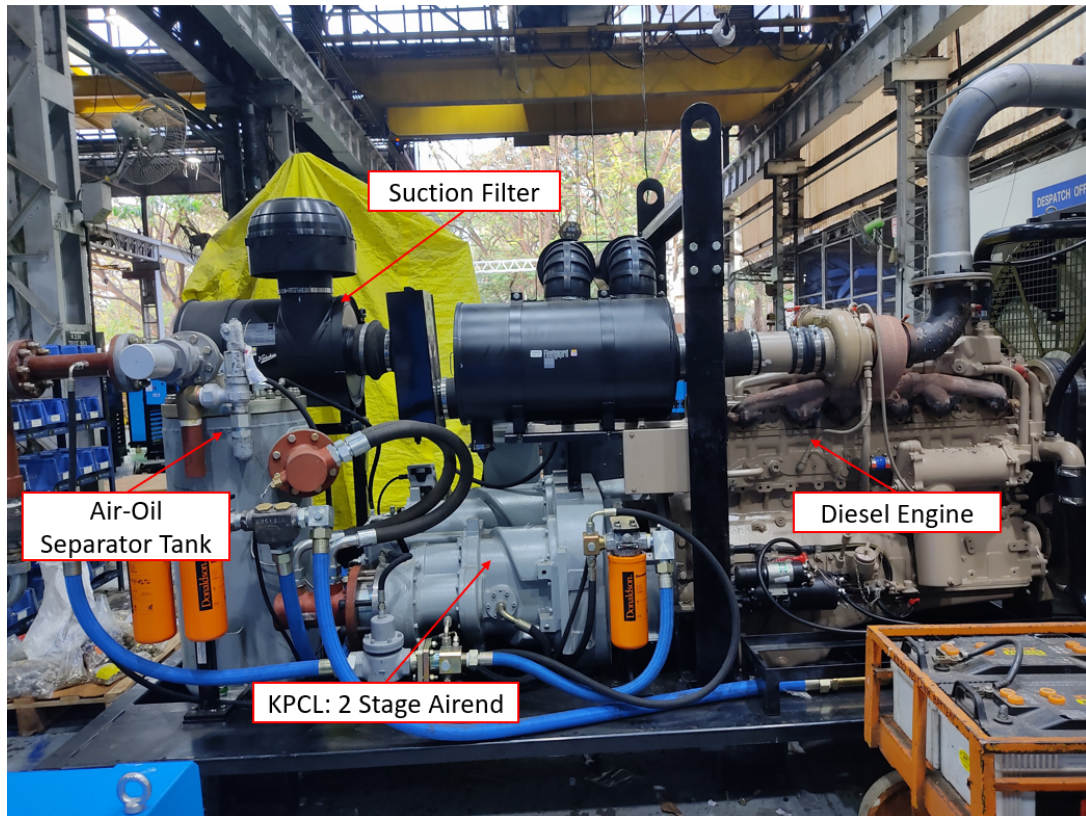


Figure 5.22: Schematic labeled diagram of the two-stage compressor test rig. The diagram illustrates the complete test rig components, including the bare two-stage KPCL compressor, providing a comprehensive view of the experimental setup.

To ensure the chamber model accurately reflects real-world compressor performance, key input parameters such as suction pressure, final discharge pressure, mass flow rate, suction temperature, and working fluid properties were incorporated into the simulations. The model was then tuned to further align with experimental data, reducing deviations and improving predictive accuracy. The chamber model was applied to three distinct discharge pressures—21.54 bar, 23.31 bar, and 25.07 bar—to validate its robustness.

Figure 5.23 illustrates the correlation between tip speed and power consumption for the low-pressure (LP) and high-pressure (HP) stages at these operating conditions. The trends obtained from the chamber model exhibit strong agreement with experimental results, demonstrating its capability as a reliable digital twin for screw compressor analysis.

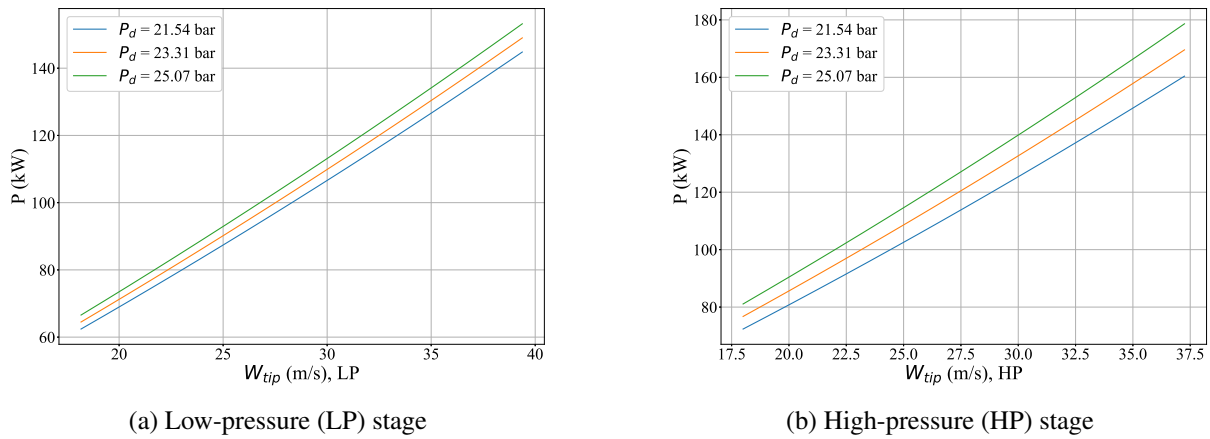


Figure 5.23: Tip speed vs. power consumption (Chamber model predictions)

Comparison with experimental data and model tuning

The chamber model predictions were compared against experimental data to evaluate their accuracy before and after fine-tuning. Initially, as illustrated in Figure 5.24a, the percentage error between the chamber model predictions and experimental results was within the $\pm 5\%$ range. While this agreement was reasonable, further refinements were made to improve accuracy.

By adjusting key model parameters—such as rotor clearances, leakages, and heat transfer coefficients—the chamber model was fine-tuned to better align with experimental observations. The updated predictions, presented in Figure 5.24b, show that the percentage error has been reduced to within $\pm 1\%$, demonstrating a significantly improved correlation with experimental data.

This refined chamber model now serves as a highly accurate digital tool for compressor performance evaluation, enabling more precise predictions and supporting the training of machine learning models with high-quality synthetic data.

5.3.8 Role of the chamber model in machine learning validation

The chamber model plays a crucial role in both performance prediction and machine learning validation. Since the chamber model accurately represents compressor behavior—validated against experimental data—it serves as a reliable digital tool for generating synthetic datasets.

In this research, the chamber model was leveraged to produce high-fidelity synthetic data,

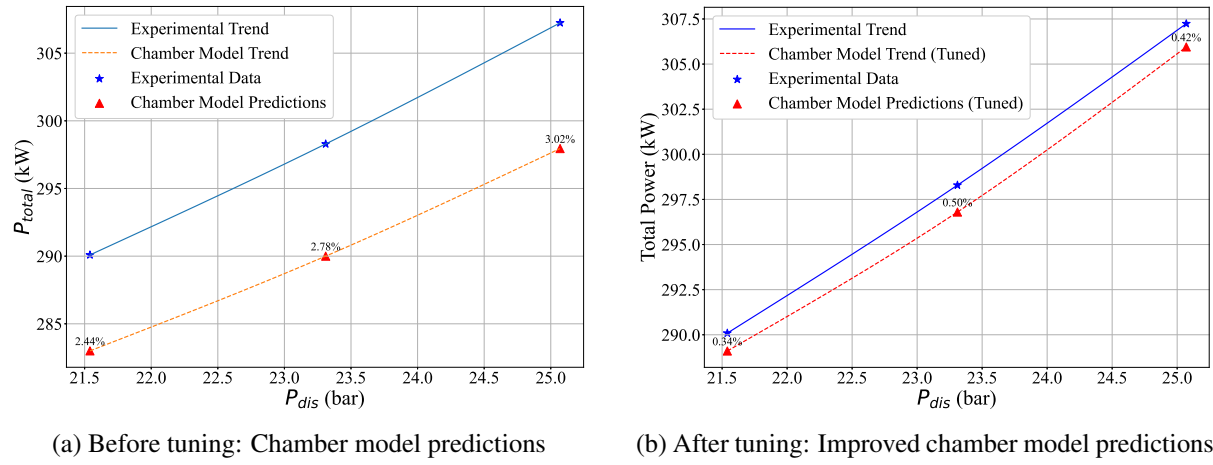


Figure 5.24: Comparison of chamber model predictions before and after tuning. Adjustments in clearances, leakages, and heat transfer coefficients led to improved agreement with experimental data, reducing percentage error from $\pm 5\%$ to $\pm 1\%$.

which was subsequently used to train the Gaussian Process Regression (GPR) model. Given the strong agreement between chamber model predictions and experimental results, the machine learning model can be validated against either real-world experimental data or chamber model outputs, as both exhibit comparable predictive accuracy.

This methodology is particularly advantageous in scenarios where experimental data is limited. By ensuring that the machine learning model is trained on well-represented compressor physics, the framework remains robust and generalizable across different operating conditions.

Validation of Gaussian Process Regression model

To assess the efficacy of machine learning in predicting compressor performance, this study employed Gaussian Process Regression (GPR). Previous research has demonstrated that GPR outperforms other machine learning models in screw compressor applications due to its ability to:

- Capture uncertainty in predictions, ensuring reliable outputs even with limited training data.
- Accurately model nonlinear interactions between input variables in multi-stage compressors.

- Generalize effectively across different compressor configurations and operating conditions.

The training dataset was derived from experimental measurements and chamber model predictions, encompassing data from 10 distinct screw compressors manufactured by KPCL, with each dataset containing at least 19,200 data points per unit. The Bayesian optimization technique was applied to fine-tune GPR hyperparameters, ensuring optimal generalization.

For validation, the dataset was split into training (80%) and testing (20%) subsets, enabling rigorous performance evaluation. The trained GPR model was then used to predict compressor power consumption and flow rate for individual stages. The GPR model predictions for LP and HP stage are shown in Figure 5.25.

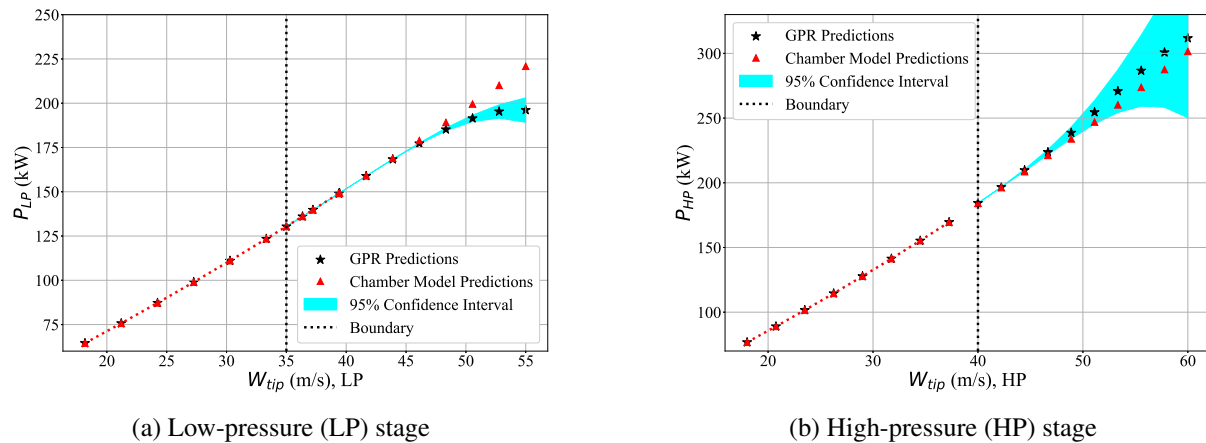


Figure 5.25: Tip speed vs. power consumption (Gaussian Process Regression predictions)

Comparison between machine learning and chamber model predictions

The predictive performance of the GPR model was assessed by comparing its outputs with both experimental data and chamber model predictions. Figure 5.26 illustrates the power consumption forecasts across different discharge pressures.

Figure 5.26 shows the total power predictions across different discharge pressures, where:

- Black star markers represent GPR model predictions.
- Red triangles denote chamber model predictions.

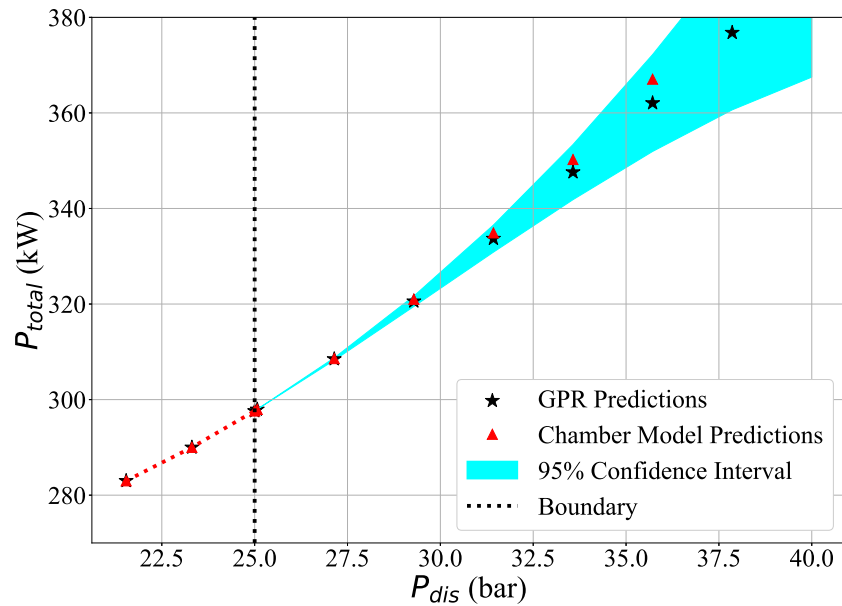


Figure 5.26: Compressor performance predictions using the GPR model for various discharge pressures in both territorial and extra-territorial regions, along with uncertainties. Predictions from the physics-based chamber model are plotted for comparison.

- The dotted boundary differentiates the territorial region (trained dataset) from the extra-territorial region (entirely unknown operational conditions).

Even in the extra-territorial region, where the model encounters unseen data, GPR predictions consistently fall within the 95% confidence interval. This highlights the model's robustness and its ability to generalize to new operating conditions.

Furthermore, the close agreement between GPR predictions and chamber model outputs reinforces the validity of using the chamber model as a digital twin for synthetic data generation. This combined approach enables reliable performance forecasting for screw compressors without requiring extensive experimental datasets.

Key Takeaways

- The chamber model was fine-tuned to match experimental data, making it a reliable source for machine learning training.
- The GPR model successfully captured compressor behavior, achieving strong agreement with both chamber model and experimental results.

- The ML model remains robust, even in extra-territorial regions, ensuring reliable performance predictions for new operating conditions.
- This hybrid approach—combining physics-based modeling with machine learning—enables more efficient screw compressor optimization and design exploration.

5.3.9 Performance optimisation of two-stage screw compressor

The optimization process was conducted using a Bayesian optimization approach within the developed modelling framework, refining critical fluid injection properties for both stages of the two-stage screw compressor. The primary objectives were to minimize the total power consumption, maximize the volumetric flow rate (Q), and reduce the specific power consumption (SPC). Through an iterative optimization approach, each parameter was adjusted to improve compressor performance, as shown in Figures 5.27(a) and 5.27(b).

The main input parameters and working fluid properties used for optimization were:

- Suction Pressure for LP Stage: Atmospheric pressure (bar)
- Final Discharge Pressure: 23 bar
- Suction Temperature: 30 °C
- Number of Stages: 2
- Working Fluid: Air
- Initial Speed of LP Stage Male Rotor: 3000 RPM

Optimisation of fluid injection parameters

The fluid injection parameters for both stages were selected as key variables due to their direct impact on the compressor's thermal and mechanical performance. In this case, oil serves as the injected fluid to cool the compression chamber, seal leakage gaps, and lubricate rotors and bearings. For screw compressors, oil contributions are typically allocated in the following proportions: cooling (100 parts), sealing (10 parts), and lubrication (1 part). Optimizing injection quantities and conditions is crucial, as excessive or insufficient oil injection can lead to additional power losses [4]. The fluid injection parameters considered in this study are detailed below:

- Oil Injection Pressure (P_{oil} in bar): This controls the flow rate of the injected oil. Higher oil flow rates improve heat exchange between the gas and oil, which can reduce discharge temperatures and enhance volumetric and adiabatic efficiency. However, excessive oil flow increases power losses due to higher resistance.

- Oil Injection Temperature (T_{oil} in $^{\circ}\text{C}$): Lower injection temperatures improve heat exchange but can add strain on the cooling system. Optimal oil temperature helps maintain balance between cooling efficiency and system load.
- Oil Injection Angle (θ in $^{\circ}$): Proper positioning of the oil injection port within the compression chamber is essential for maximizing heat transfer. An injection point closer to the discharge port limits residence time for heat transfer, while a point closer to the suction side enhances cooling efficiency.
- Oil Injection Port Diameter (D_{oil} in mm): This influences oil flow rate and pressure losses. An optimal port diameter minimizes frictional losses while ensuring adequate cooling, preventing thermal deformation.

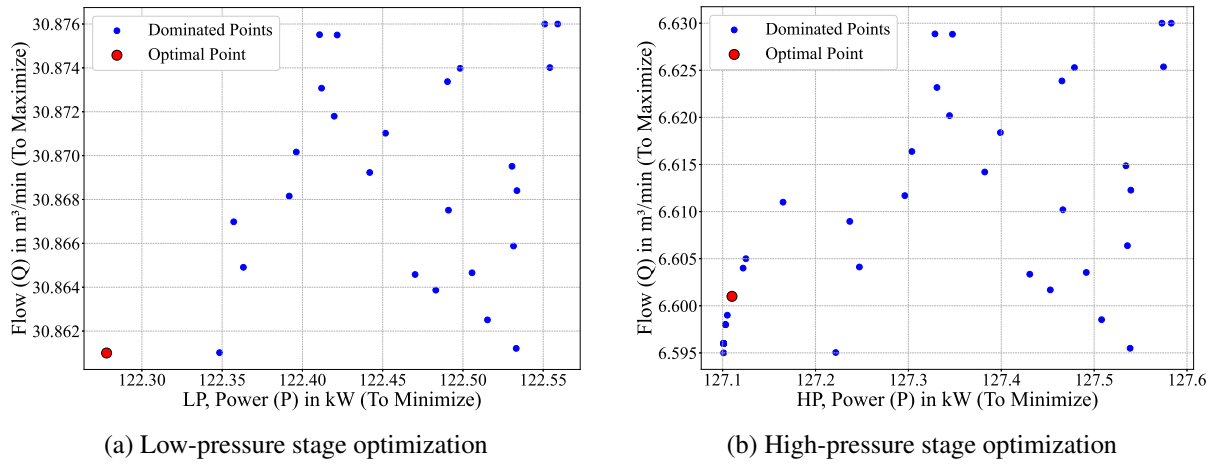


Figure 5.27: Pareto Fronts illustrating the trade-offs between power and flow rate for (a) low-pressure stage and (b) high-pressure stage achieved through fluid injection parameter optimization.

Optimized parameters and performance results

The optimized parameters for both stages are presented in Table 5.9. Significant improvements were observed due to optimized fluid injection, which positively influenced the compressor's overall efficiency.

The results, shown in Table 5.10, highlight the performance improvements achieved. Total power consumption was reduced by 1.2%, with a nearly 2% reduction in specific power consumption (SPC), enhancing system energy efficiency. The volumetric flow rate (Q) saw a slight increase of approximately 0.8%, indicating improved system capacity.

Table 5.9: Optimized Fluid Injection Parameters for Two-Stage Screw Compressor

Parameter	Range (LP & HP)	Optimized Value (LP)	Optimized Value (HP)
P_{oil} (bar)	18 - 23	19	19
T_{oil} (°C)	40 - 90	40	44
D_{oil} (mm)	4 - 20	12	11
θ (°)	30 - 150	122	76

Table 5.10: Comparative Analysis of Two-Stage Compressor Performance Optimization

Performance Parameter	Original Value	Optimized Value	% Change
Total Power (kW)	252	249	1.2%
SPC (kW/m ³ /min)	8.218	8.057	2.0%
Q (m ³ /min)	30.664	30.903	0.8%

Interpretation of results

The optimised oil injection pressure of 19 bar, together with oil port widths of 12 mm for the low-pressure stage and 11 mm for the high-pressure stage, enhanced the flow rate and decreased the discharge temperature. Injection at roughly 40 °C facilitated efficient heat exchange without overburdening the cooling system. Moreover, oil injection angles of 122° for the LP stage and 76° for the HP stage ensured adequate residence time for heat transmission, with injection sites strategically positioned to enhance chamber temperature management.

These optimisations collectively yielded a 2% enhancement in system efficiency. The modified injection parameters reduced frictional losses and enhanced cooling and sealing effects, illustrating that meticulous regulation of fluid injection characteristics is essential for performance improvements.

This optimisation case study underscores the efficacy of the modelling tool in enhancing power and flow parameters. Nevertheless, in practical implementations, factors such as customer-specified flow requirements or power limitations imposed by the motor or drive system must be taken into account to ensure conformity with operational demands and system efficiency requirements.

5.4 Summary

This chapter introduced a comprehensive framework for the prediction and optimisation of screw compressor performance, with a specific focus on multi-stage configurations. The framework integrates traditional chamber models with advanced Machine Learning (ML) techniques, leveraging Gaussian Process Regression (GPR) for accurate performance prediction and Bayesian Optimisation for parameter tuning.

Experimental validation of the framework demonstrated its reliability, with predictions for power consumption and performance metrics falling within an acceptable error margin of $\pm 5\%$. This level of accuracy underscores the framework's capability to predict screw compressor performance across various operating conditions, while also addressing key challenges such as uncertainty quantification.

Key advancements included the optimisation of fluid injection parameters for a two-stage screw compressor, achieving a 2% reduction in specific power consumption and a marginal improvement in volumetric flow rate. The optimisation process illustrated the potential of the framework to improve efficiency and reliability in high-pressure applications.

The framework provides significant computational advantages over traditional thermodynamic solvers, enabling rapid and efficient performance predictions for both single-stage and multi-stage compressors. Furthermore, the experimental validation confirmed the accuracy and applicability of the model in industrial scenarios, particularly for the optimisation of compressor parameters such as intermediate pressure, built-in volume ratio, and fluid injection settings.

Future research will focus on expanding the dataset to include additional compressor sizes, enhancing the generalisability of the GPR-based solver, and integrating real-world constraints such as customer-specific flow requirements and power limitations. These efforts aim to further refine the modelling framework and ensure its suitability for diverse industrial applications.

Chapter 6

Economic Analysis of Multi-Stage Screw Compressors

The literature offers significant insights into the performance and efficiency of multi-stage screw compressors; nonetheless, there exists a notable deficiency in studies concerning the economic assessment of multi-stage compared to single-stage systems in medium-pressure applications. Most research emphasises high-pressure applications, when multi-stage systems are the evident selection. This research enhances the field by concentrating on medium-pressure applications (6-12 bar) with power ratings between 22 and 315 kW, a domain where the advantages of multi-stage compressors are inadequately documented. This study offers actual proof of the economic feasibility of two-stage systems in medium-pressure environments through a comprehensive lifecycle cost analysis. The study presents a prototype two-stage oil-flooded screw compressor, specifically engineered for water well applications, which has undergone performance and reliability testing and evaluation.

This research is innovative due to its thorough methodology in enhancing the efficiency of two-stage screw compressors for medium-pressure applications. This study boosts compressor performance and illustrates the long-term cost savings of two-stage systems through the integration of current rotor profiles, innovative sealing technologies, and efficient cooling systems. The results demonstrate that two-stage compressors can save operational expenses by 20-75%, contingent upon the power rating and application, rendering them an attractive alternative to single-stage systems in medium-pressure contexts [5].

6.1 Design and sizing of screw compressor systems

This study concentrates on the design and optimisation of a two-stage oil-flooded air screw compressor system. The choice to restrict the investigation to two stages is predicated on the intrinsic limits of screw compressors at elevated pressure stages. In high-pressure stages, the rotor dimensions are diminished, resulting in decreased tip velocities and, subsequently,

a reduction in efficiency. Moreover, the ratio of oil volume to gas volume increases at elevated pressures, hence diminishing performance. Consequently, screw compressors beyond two stages are typically not favoured in industrial applications.

The main aim of this research is to determine the ideal dimensions for two-stage oil-flooded air screw compressors, using data from 7 distinct single-stage compressor sizes produced by Kirloskar Pneumatic Company Limited (KPCL), Pune, India. The appropriate sizing was established with an internally created modelling tool that combines a chamber model with machine learning approaches to precisely forecast compressor performance while optimising computational efficiency [50, 9].

After determining the ideal dimensions for the low-pressure (LP) and high-pressure (HP) phases, a thorough economic analysis was performed. This comparison was founded on essential performance parameters and the subsequent power ratings (see to Table 6.1). The investigation was confined to an 8.5:1 pressure ratio utilising oil injection and air as the working fluid to maintain uniformity in the comparison. The study emphasises these factors; nonetheless, it is noteworthy that two-stage screw compressors can attain discharge pressures of up to 30 bar, contingent upon application requirements. The prototype two-stage compressor, created for this research, was engineered to achieve a final pressure of 25 bar for experimental validation.

A conventional two-stage screw compressor system comprises two compressor blocks of varying sizes, linked by an intermediate pipe that serves as an intercooler, akin to reciprocating compressors. The system has a gear configuration with a bull gear and two pinions affixed to the LP and HP male rotors. The rotors are powered by a singular motor, guaranteeing effective functioning across both stages.

Table 6.1 outlines the technical parameters of the single-stage oil-flooded compressor blocks employed in this study, each with a 4/5 lobe configuration and a length ratio of 1.55. KAS-350 is the sole compressor block featuring a 4/6 lobe configuration with a relative length of 1.65. Confidentiality agreements restrict the revelation of precise rotor measurements and specific technical information. The compressor blocks are identified as KAS, with the number indicating the specific compressor model.

A proprietary modelling technique was employed to ascertain the ideal dimensions for a two-stage screw compressor based on the existing single-stage sizes. The architectural framework of this tool is depicted in Figure 6.1. The tool employs a robust modelling framework that incorporates either the chamber model or Gaussian Process Regression (GPR) model, contingent upon the required accuracy and computing efficiency. This methodology guarantees that

Table 6.1: Power ratings, pressure ratio, flow for single-stage compressor blocks, and optimal two-stage combinations.

Power Rating (kW)	Single-Stage Compressor Block	Pressure Ratio	Flow (m^3/min)	Best Optimal Combination (LP / HP)
22	KAS-200	8.5	3.57	LP: KAS-200 / HP: KAS-100
37	KAS-300	8.5	7.11	LP: KAS-300 / HP: KAS-200
55	KAS-500	8.5	10.85	LP: KAS-400 / HP: KAS-350
75	KAS-500	8.5	15.12	LP: KAS-400 / HP: KAS-350
90	KAS-500	8.5	17.92	LP: KAS-400 / HP: KAS-350
110	KAS-500	8.5	21.78	LP: KAS-500 / HP: KAS-350
132	KAS-500	8.5	24.95	LP: KAS-500 / HP: KAS-350
160	KAS-500	8.5	29.65	LP: KAS-500 / HP: KAS-350
315	KAS-650	8.5	57.57	LP: KAS-500 / HP: KAS-350

the modelling process complies with essential boundary conditions vital for precise forecasts of multi-stage compressor performance:

- **Mass Conservation Across All Stages:** The mass conservation principle ensures that the mass flow rate remains consistent across all stages, guaranteeing that no mass is lost or artificially created throughout the compression process.

$$\dot{m}_{in,i} = \dot{m}_{out,i} \quad (6.1)$$

Where: $\dot{m}_{in,i}$ is the mass flow rate entering stage i , and $\dot{m}_{out,i}$ is the mass flow rate exiting stage i .

- **Intermediate Pressure Balance:** The intermediate pressure, acting as the discharge pressure for the low-pressure (LP) stage and the suction pressure for the high-pressure (HP) stage, must be carefully balanced to optimize the performance of the system. The optimal intermediate pressure (P_i) can be calculated as the geometric mean of the suction pressure (P_1) and the discharge pressure (P_2):

$$P_i = \sqrt{P_1 \cdot P_2} \quad (6.2)$$

This equation shows that for a multi-stage screw compressor, the minimum power occurs when the intermediate stage pressure is the geometric mean of the suction and discharge pressures. In the case of systems with multiple stages, the pressure ratio for each individual stage should be balanced to minimize power consumption. For a compressor with N stages, the optimal stage pressure ratio is given by:

$$\text{Individual stage pressure ratio} = \sqrt[N]{\frac{P_2}{P_1}} \quad (6.3)$$

This formula helps to determine the optimal pressure ratios for each stage, ensuring the overall system operates efficiently by minimizing the required power for compression. While ideal conditions assume that the intermediate pressure remains constant, minor pressure drops may occur due to system inefficiencies, such as losses in the interstage piping or heat transfer during compression.

- **Intermediate Temperature Balance:** The intermediate temperature, representing the discharge temperature of the LP stage and the suction temperature of the HP stage, is expected to be equal. Any potential temperature reductions are primarily due to inter-cooling effects in the connecting pipes.

The aforementioned boundary requirements are crucial for preserving the thermodynamic consistency of the system. The modelling framework assesses these conditions in the background to guarantee the proper configuration of the compressor stages. The instrument employs a blend of optimisation methodologies and performance simulations to determine the most effective configuration of LP and HP stages, as shown in Table 6.1.

Figure 6.1 illustrates the architecture utilised in the modelling tool. The framework is designed to permit the adaptable choice of the physics solver—either the chamber model or a machine learning-based solver, contingent upon the study’s requirements. This adaptability guarantees that the tool can be utilised in many contexts, from swift initial assessments to comprehensive performance enhancements.

The modelling tool finally produces essential performance metrics including efficiency, power consumption, and mass flow rate. These results offer critical insights into the optimal design and performance of two-stage screw compressors, guaranteeing that the system is both technically and economically feasible for diverse applications.

6.2 Analysis of lifecycle costs for different compressor systems

The lifecycle costs of a compressor system include initial capital expenditure, operating expenses (mostly energy consumption), maintenance costs, installation costs, and disposal costs. Each of these criteria is essential in ascertaining the total cost of ownership during the system’s operating lifespan.

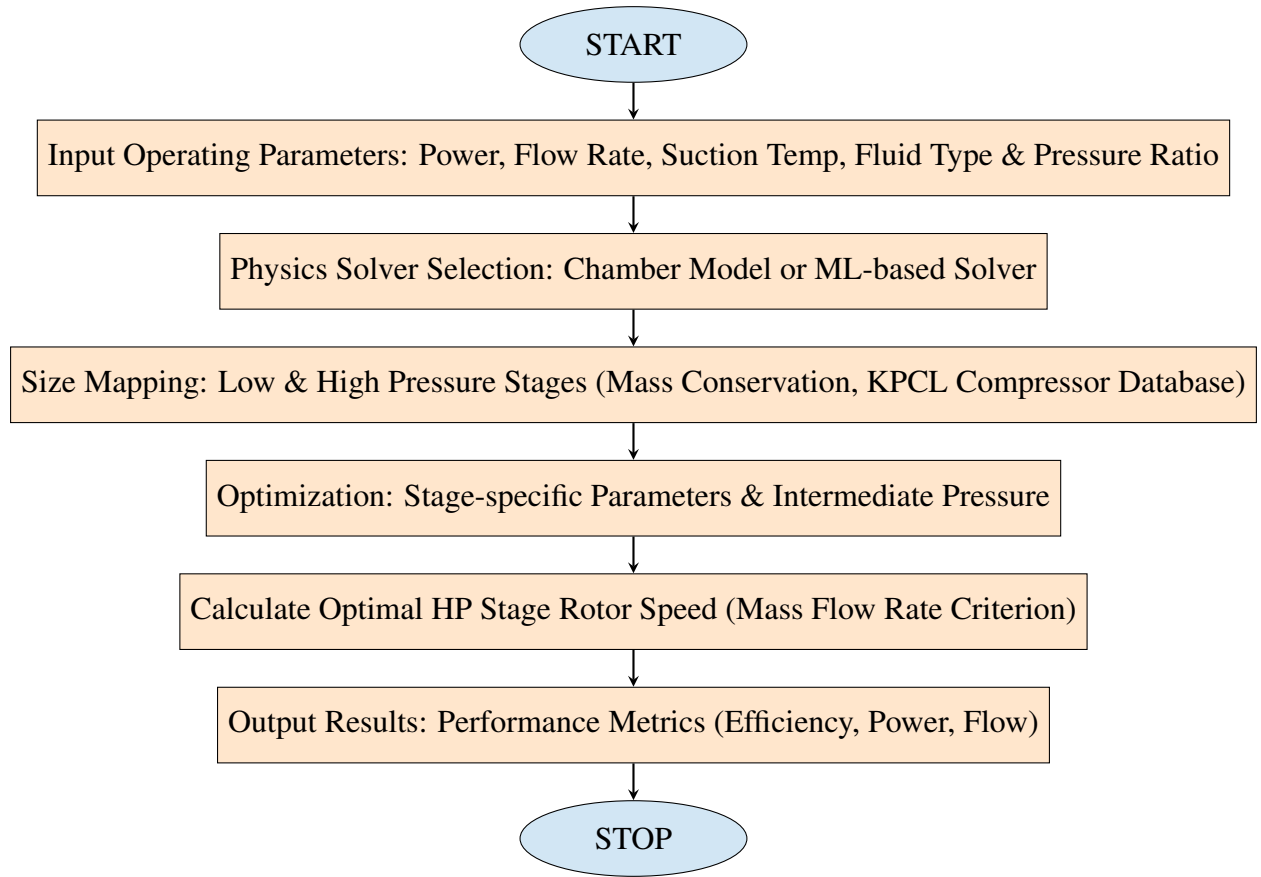


Figure 6.1: Modeling framework architecture for optimizing two-stage screw compressors and individual stage parameters using a chamber model and machine learning-based approach.

Disposal costs, determined by the materials utilised in compressor construction, are presumed to be identical for both single-stage and two-stage systems of equivalent size. Since disposal costs remain relatively consistent across all configurations in this analysis, they will not be discussed further.

The cost data obtained from Kirloskar Industry cannot be released due to confidentiality agreements. All costs are instead shown as normalised values for the sake of comparison. The normalisation method preserves the relative disparities between single-stage and two-stage systems while ensuring data confidentiality.

The cost normalisation adheres to the following formula:

$$C_{\text{normalized}} = \left(\frac{C_{\text{two-stage}} - C_{\text{single-stage}}}{C_{\text{single-stage}}} \right) \times 100 \quad (6.4)$$

Where:

- $C_{\text{normalized}}$ is the percentage difference in cost,
- $C_{\text{two-stage}}$ is the cost of the two-stage compressor (e.g., operating, maintenance, or lifecycle cost),
- $C_{\text{single-stage}}$ is the cost of the single-stage compressor, used as the reference value.

This normalisation method facilitates a more transparent comparison of lifecycle costs among various compressor systems while safeguarding confidential financial information.

The cost normalisation is determined by referencing the lifecycle cost of a single-stage compressor with the same power rating as the two-stage compressor under evaluation. For instance, when calculating the lifecycle cost of a two-stage compressor with a power rating of 22 kW, the corresponding lifecycle cost of a single-stage compressor with a 22 kW power rating is used as the baseline. This approach ensures consistency in comparisons across all power ratings, as detailed in Table 6.1.

To further clarify the systems under evaluation, Figure 6.2 provides a schematic of a screw compressor system. This configuration applies to both single-stage and two-stage compressors, highlighting essential components such as the screw compressor block, motor, air-oil separator, and air delivery system. Such a system forms the basis for the lifecycle cost comparisons in this study.

6.2.1 Initial costs

The initial expense of two-stage compressors typically exceeds that of single-stage compressors. The cost disparity is due to the intricate design and supplementary components associated with two-stage systems. In contrast to single-stage compressors, which have a singular compression unit, two-stage compressors feature two distinct compression stages. This encompasses:

- **Two compression units:** In a two-stage system, there exist two separate compressors, each comprising its own rotor and housing. The redundancy of compression hardware results in a direct escalation of material and production expenses.

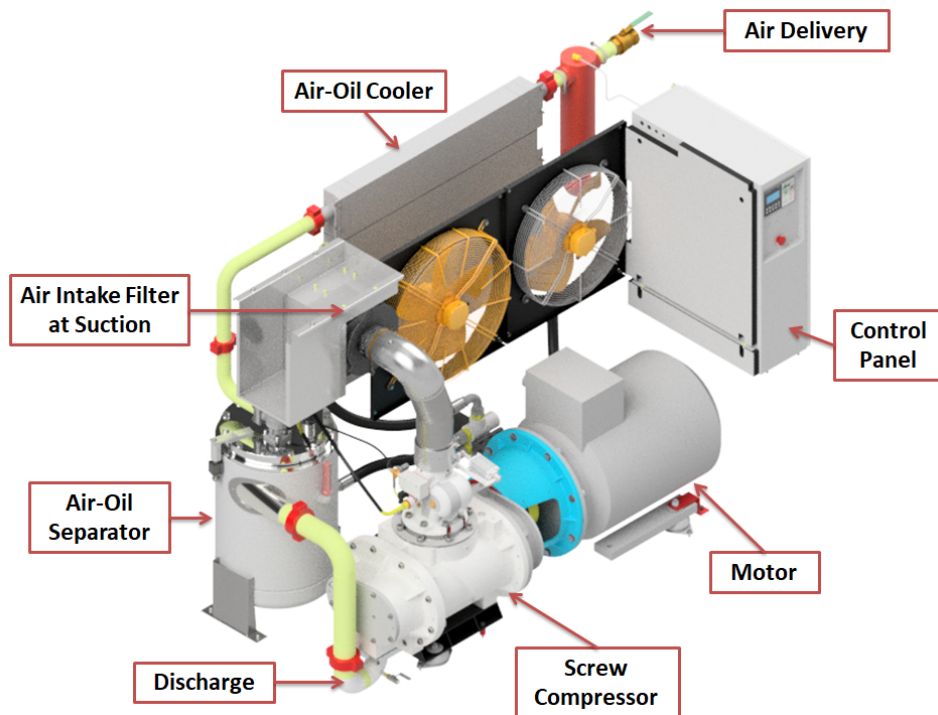


Figure 6.2: Schematic representation of a screw compressor system illustrating key components, including the air-oil cooler, control panel, air-oil separator, motor, and discharge system. This configuration can represent either a single-stage or two-stage screw compressor system, commonly used in various industrial applications for compressing air or gas.

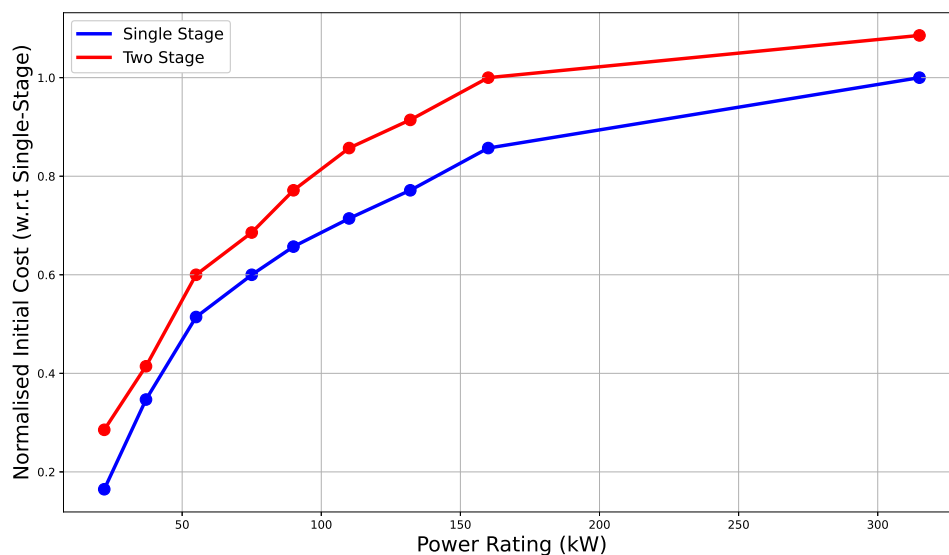


Figure 6.3: Normalised initial cost comparison between single-stage and two-stage compressors across the power range of 22 to 315 kW.

- **Interstage piping and intercooler:** The two compression stages are linked by an interstage pipe, which frequently serves as an intercooler. This supplementary component adds complexity and expense due to the requirement for meticulous design and integration to efficiently regulate temperature and pressure between stages.
- **Bull gear arrangement:** In a dual-stage system, a bull gear mechanism is commonly utilised to operate both the low-pressure (LP) and high-pressure (HP) compressors. This gear configuration enables a single motor to drive both stages, augmenting the mechanical complexity of the system and hence elevating the initial cost.
- **Additional cooling and sealing systems:** The elevated operating pressures and temperatures associated with two-stage compression need the implementation of more durable cooling and sealing systems. These systems augment the total expense by necessitating specialised components and engineering expertise.

The cumulative impact of these considerations leads to a greater initial expenditure for two-stage compressors relative to single-stage models. Figure 6.3 depicts the normalised initial cost comparison between single-stage and two-stage compressors.

6.2.2 Operating costs

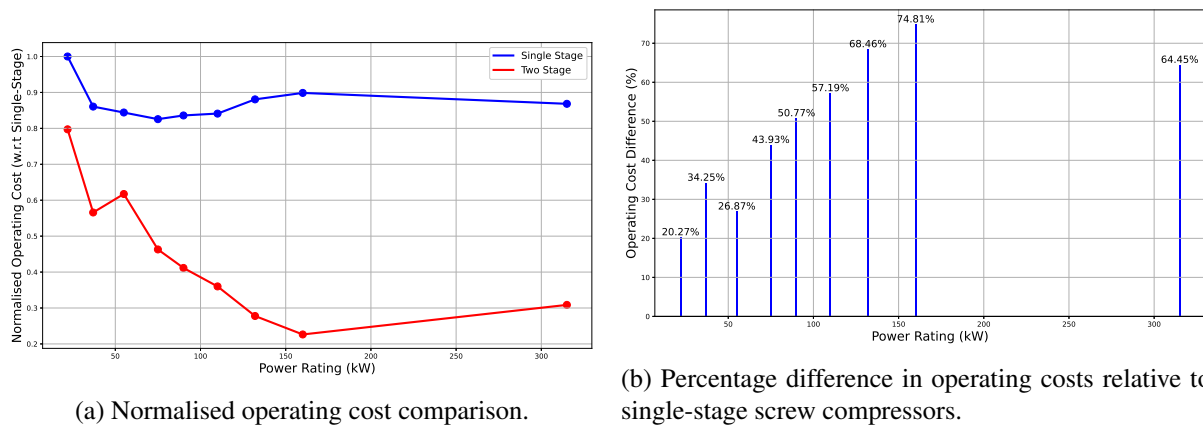


Figure 6.4: Comparison of operating costs for single-stage and two-stage compressors across power ratings from 22 to 315 kW.

The operating cost of compressors is a critical factor in their overall lifecycle costs, and it is calculated based on the specific power consumption (SPC), the total operating hours, and the cost of energy per unit of consumption. The operating cost formula is given as:

$$C_{\text{operating}} = SPC \times H \times C_{\text{energy}} \quad (6.5)$$

Where:

- $C_{\text{operating}}$ is the total operating cost over the compressor's lifetime,
- SPC is the specific power consumption of the compressor in $kW/m^3/min$,
- H is the total operating hours, which is calculated based on 22 hours of operation per day for 10 years (i.e., $H = 22 \times 365 \times 10$ hours),
- C_{energy} is the cost of energy per unit (in INR or other currency).

The power consumption differs between single-stage and two-stage compressors, with two-stage compressors typically exhibiting greater energy efficiency, especially at elevated power ratings. The normalised operating cost comparison illustrated in Figure 6.4a indicates a substantial decrease in operating costs for two-stage compressors across all power ratings. The trend becomes increasingly apparent with higher power ratings, and the specific power consumption of two-stage systems enhances their performance.

For lower power ratings, such as 22 kW and 37 kW, the cost reduction is very modest, indicating the incremental efficiency improvements realised by two-stage compressors under reduced pressure settings. Nonetheless, for mid-range power ratings (75 kW, 90 kW, and 110 kW), the reduction in running costs becomes increasingly evident. This is due to the improved efficiency of two-stage compressors, which manage elevated pressures more effectively and gain from superior cooling between stages.

At elevated power ratings, specifically 160 kW and 315 kW, the energy savings linked to two-stage compressors are significantly greater. This is chiefly because to their capacity to sustain reduced specific power consumption, hence considerably diminishing energy usage during prolonged operational durations. With a rise in power rating, the efficiency improvements and operational cost savings of two-stage compressors become progressively beneficial.

Figure 6.4b further depicts the % disparity in operating expenses between single-stage and two-stage compressors with a bar graph. This visual depiction distinctly shows the escalating benefits of two-stage systems as the power rating rises.

6.2.3 Lifecycle costs

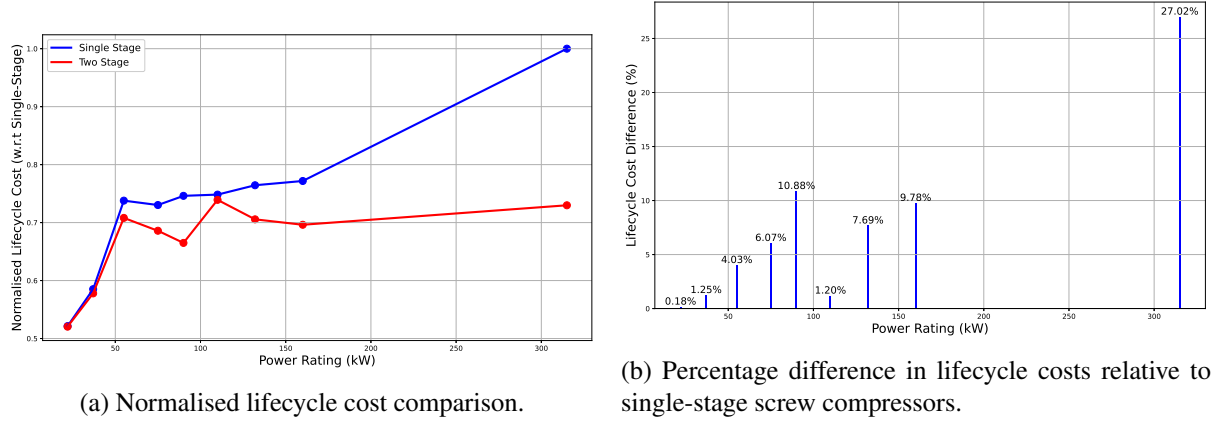


Figure 6.5: Comparison of lifecycle costs for single-stage and two-stage compressors across power ratings from 22 to 315 kW.

The lifecycle cost of a compressor system denotes the aggregate ownership expense during its operational duration, generally assessed over a term of 10 years. The lifecycle cost is calculated by aggregating the initial capital cost, maintenance cost, installation cost, operating cost, and disposal cost. The lifecycle cost for this analysis is determined using the subsequent formula:

$$C_{\text{lifecycle}} = C_{\text{initial}} + C_{\text{maintenance}} + C_{\text{installation}} + C_{\text{operating}} + C_{\text{disposal}} \quad (6.6)$$

Where:

- $C_{\text{lifecycle}}$ is the total lifecycle cost over the 10-year operating period,
- C_{initial} is the initial or capital cost of the compressor system,
- $C_{\text{maintenance}}$ is the cost of maintaining the system over the 10 years,
- $C_{\text{installation}}$ is the installation cost,
- $C_{\text{operating}}$ is the operating cost, calculated based on specific power consumption, operating hours, and energy cost,
- C_{disposal} is the disposal cost at the end of the system's operational life.

This study concentrates on the primary factors influencing lifetime costs: capital cost, operational cost, and lifecycle cost. Minor contributions, including maintenance, disposal, and installation expenses, are not specifically detailed but are incorporated into the overall lifecycle calculation.

Figure 6.5a depicts the comparative analysis of normalised lifespan costs for single-stage and two-stage compressors. Similar to operating expenses, two-stage compressors exhibit a cost benefit, especially when the power rating escalates. The percentage decrease in lifetime costs is less significant than that of operating expenses, as the initial capital investment for two-stage compressors is elevated due to increased complexity and more components.

The percentage decrease in lifespan costs for two-stage compressors, relative to single-stage compressors, fluctuates with power rating. Figure 6.5b illustrates the trend in lifespan cost reduction across different power ratings:

- At lower power ratings, such as 22 kW and 37 kW, the lifecycle cost reduction is modest at approximately 0.18% and 1.25%, respectively. This reflects the smaller difference in efficiency and capital investment at lower power levels.
- In the mid-range power ratings (55 kW, 75 kW, 90 kW), the lifecycle cost reduction becomes more significant, with values of up to 10.88% at 90 kW. This is attributed to the increased efficiency of two-stage compressors and the ability to handle higher pressure ratios, which leads to lower operating costs over time.
- For higher power ratings, such as 160 kW and 315 kW, the lifecycle cost savings become even more pronounced, reaching up to 27.02% at 315 kW. This is a direct result of the substantial energy savings achieved by two-stage compressors at these higher capacities, despite the initial capital cost being higher.

The bar graph in Figure 6.5b clearly illustrates the disparity in lifespan costs between single-stage and two-stage compressors, with the cost benefit becoming increasingly evident as power ratings rise.

The lifecycle cost analysis presented in this study has been conducted considering economic conditions prevailing in *India*, including *energy tariffs*, *labor costs*, and *maintenance expenses*. These factors can vary significantly across different regions, influencing the share of operating and maintenance costs in the total lifecycle cost. As a result, the economic feasibility and optimal operating conditions for single-stage and two-stage compressor systems are highly

region-dependent. Future research may extend this analysis by incorporating global variations in energy pricing, labor rates, and taxation structures to offer a broader perspective on lifecycle cost assessment.

To validate the theoretical outcomes and the lifecycle cost analysis outlined in *Section 5.3.6*, a prototype of a two-stage air screw compressor was designed and manufactured for water-well applications. Following initial performance testing, the compressor underwent a comprehensive in-house evaluation for approximately 150 hours to ensure its compliance with design specifications and industry standards, including ISO 1217 (displacement compressor evaluation) and ISO 5389 (performance assessment). The experimental setup is depicted in *Figure 5.22*. These standards guarantee the accuracy of airflow, pressure, and power consumption measurements under real-world operating conditions.

Upon successful validation, the prototype was deployed at a client location, where it has been operating consistently for *over a year*. This extended operational period has provided valuable empirical data, demonstrating the durability and economic advantages of the two-stage system. The reduction in lifecycle costs, primarily due to lower specific power consumption and higher efficiency at elevated discharge pressures, aligns with the findings of this study. The distribution of lifecycle costs over the one-year evaluation period is illustrated in *Figure 6.6*, emphasizing the contribution of each cost component.

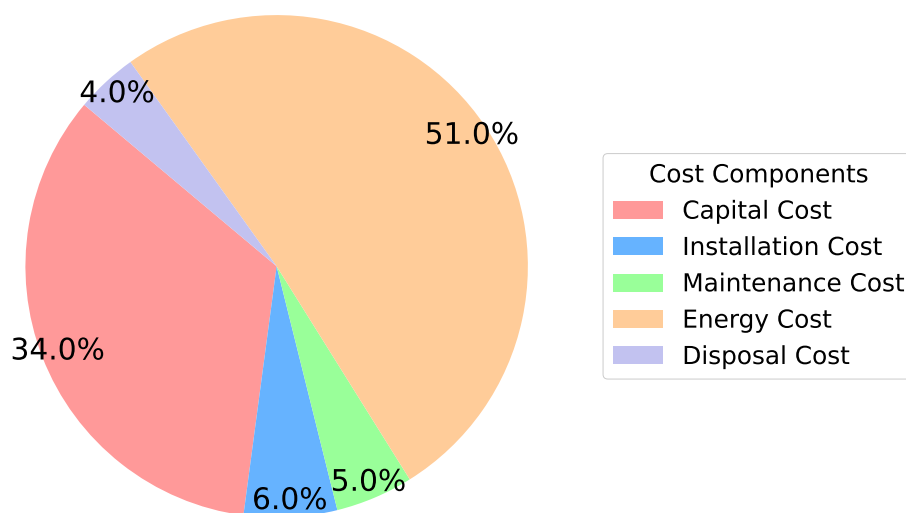


Figure 6.6: Lifecycle cost breakdown of a two-stage oil-flooded air screw compressor system with a 307 kW power rating and 25 bar discharge pressure, based on one year of operation.

The experimental results, along with the lifetime cost evaluation, demonstrate that two-stage screw compressors are both feasible and economically beneficial for high-pressure discharge applications, such as water-well systems. Empirical evidence substantiates the conclusions derived from modelling and analysis, providing a compelling rationale for the lifecycle cost savings realised by two-stage systems.

6.3 Summary

This research provided an exhaustive analysis of the lifecycle costs related to single-stage and two-stage screw compressors, emphasising the economic advantages of two-stage systems. The research included theoretical modelling, lifecycle cost analysis, and practical validation to emphasise the benefits of two-stage screw compressors for operational cost reduction and overall efficiency, especially in high-pressure applications.

The findings demonstrate that although two-stage compressors need a greater initial capital outlay, their lower specific power consumption and enhanced efficiency at elevated discharge pressures lead to substantial operational cost reductions. The savings are more significant at elevated power ratings, as evidenced by experimental results, where a two-stage prototype functioned for almost a year, realising considerable lifecycle cost reductions. The experimental data, certified per ISO 1217 and ISO 5389 standards, substantiates the results derived from the theoretical analysis. The lifespan cost distribution of the evaluated compressor underscores the significance of operating expenses as a pivotal element in achieving long-term cost savings.

Future endeavours should focus on the creation of an optimised two-stage compressor prototype designed for an 8.5 bar discharge pressure. This prototype will have optimised compressor dimensions and an integrated volume ratio (VI) specifically engineered to provide economic advantages at reduced pressures. The objective is to transfer the economic benefits observed in high-pressure systems to mid-range pressure applications by optimising design parameters for enhanced efficiency and reduced operating expenses. Utilising the results of this study, the subsequent development phase seeks to attain optimal economic efficiency, rendering two-stage compressors a more appealing option for a broader spectrum of industrial applications.

Chapter 7

Conclusions and Recommendation for Future Work

7.1 Conclusions

This research has contributed to the modelling, optimisation, and economic analysis of screw compressors, with a focus on multi-stage configurations. The key findings are summarised as follows:

- **Optimisation of Screw Compressor Performance:** Two optimisation methodologies - Evolutionary (Genetic Algorithm) and Probabilistic (Bayesian)—were applied to refine screw compressor performance. The optimisation of KAS-300 profile clearances resulted in an estimated 33% improvement in specific power consumption, while water injection as an alternative to oil demonstrated a 4.59% improvement for KAS-200. These results indicate that advanced optimisation techniques can enhance efficiency under certain conditions.
- **Development of a Multi-Stage Compressor Modelling Framework:** A modelling framework integrating two physics solvers—Chamber Model and Machine Learning-based Gaussian Process Regression (GPR)—was developed to predict compressor performance. The ML-based model for single-stage compressors achieved high accuracy, with predictions generally within a $\pm 5\%$ margin of error when validated experimentally. The framework provides a structured approach for performance assessment.
- **Experimental Validation and Economic Analysis:** A prototype two-stage, oil-flooded air screw compressor was designed, manufactured, and tested. The economic analysis showed that while two-stage compressors have a higher initial cost, their operating costs were found to be 20-75% lower than single-stage compressors, contributing to lower lifecycle costs over a 10-year period. These results highlight the potential economic advantages of two-stage compressors in specific industrial applications.

- **Accuracy and Applicability of the Developed Models:** The chamber model and ML-based approach both demonstrated good agreement with experimental data, with predictions generally within $\pm 5\%$. While the chamber model is based on thermodynamic principles, the Bayesian Optimisation-GPR model provided an alternative data-driven approach, showing reliable predictive capabilities for both single and multi-stage compressors.
- **Multi-Stage Modelling and Fluid Injection Considerations:** The ML-based framework was extended to multi-stage compressors, indicating that optimising fluid injection parameters could improve specific power consumption by approximately 2%. This suggests that data-driven approaches could supplement traditional compressor design methodologies.
- **Limitations and Future Scope:** The study identified certain limitations, such as the sensitivity of machine learning models to data quality and the challenges in generalising predictions to unseen operational conditions. Additionally, while interstage pressure was considered as a fixed parameter based on geometric mean assumptions, future studies should investigate its dynamic optimisation to minimise overall power consumption.
- **Implications for Industry and Future Research:** The findings provide insights into screw compressor optimisation and highlight potential areas for further development. Future work could focus on refining machine learning models, incorporating real-time adaptive control, and exploring interstage pressure as an optimisation variable to improve overall system efficiency.

This research contributes to the ongoing efforts in advancing screw compressor technology. While the results demonstrate the potential for improved performance and efficiency, further experimental validation and real-world applications are needed to fully assess their industrial impact. The study provides a foundation for future investigations into optimisation techniques, modelling accuracy, and the broader economic feasibility of multi-stage screw compressors.

7.2 Future recommendations

This thesis has developed a systematic approach for the optimisation, modelling, and economic evaluation of multi-stage screw compressors. While the findings provide significant advancements in these areas, further research is needed to enhance the framework's applicability and effectiveness. The following key recommendations outline future research directions:

- **Enhancing the Optimisation Approach for Broader Applications:** The tailored optimisation approach developed in this research can be further refined by exploring additional global optimisation techniques, such as reinforcement learning and hybrid meta-heuristics. These methods could improve the framework's adaptability for different compressor configurations, operating conditions, and industrial applications beyond screw compressors.
- **Modelling Framework with Real-Time Adaptive Learning and Interstage Pressure Optimisation:** The modelling framework can be extended to incorporate real-time data acquisition and adaptive machine learning. By integrating online learning techniques, the framework could dynamically update its predictions based on operational feedback, allowing for real-time performance optimisation and improved robustness across varying conditions. Furthermore, the interstage pressure, which was assumed as a geometric mean with a fixed pressure drop for computational feasibility, should be optimised dynamically. Future work should explore interstage pressure as an independent optimization variable to achieve minimum total power consumption under varying discharge pressures and operating conditions. This could be particularly beneficial for applications where independent control of interstage parameters is feasible.
- **Expanding the Economic Analysis for Lifecycle Cost Optimization:** Future studies should extend the economic assessment by considering additional cost factors such as maintenance, part degradation, and reliability-based optimisation. A more detailed lifecycle analysis would provide deeper insights into the long-term financial benefits of multi-stage screw compressors, helping industries make more informed investment decisions.

By addressing these areas, future research can further strengthen the effectiveness of screw compressor optimisation, making it more efficient, adaptable, and economically viable for industrial applications.

List of Publications

The academic contributions made during the time this study was carried out are listed below:

Patent

1. “A System and Process for Optimization of Multi-Stage Screw Compressors”, Indian Patent Application No. 202521027574, filed in 2025. (Status: Application filed and under examination)

Journal Articles

1. **Kumar, A.**, Patil, S., Kovacevic, A. and Ponnusami, S.A., 2024. Performance prediction and Bayesian optimization of screw compressors using Gaussian Process Regression. *Engineering Applications of Artificial Intelligence*, 133, p.108270.
2. **Kumar, A.**, Kovacevic, A. and Stosic, N., 2025. Lifecycle cost analysis and performance evaluation of multi-stage screw compressors. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, p.09544062241312875.
3. **Kumar, A.**, Chaudhari, A., and Patel, D.D., 2025. Optimization, Simulation and Computational Fluid Dynamics Analysis of Oil Cooling System for Air Centrifugal Compressor. *Engineering Research Express*.
4. **Kumar, A.**, Chaudhari, A., and Patel, V.B., 2025. Optimizing tooth count in labyrinth seals for enhanced efficiency and reduced leakage in centrifugal compressors: a computational fluid dynamics study. *Sādhana - Academy Proceedings in Engineering Sciences*. (Status: Accepted for publication)

5. **Kumar, A.**, 2025. Influence of screw parameters and fluid injection on the performance of screw compressors. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*. (Status: Response to reviewer's comments submitted, under "Awaiting Decision")
6. **Kumar, A.**, Ponnusami, S.A., and Kovacevic, A., 2025. Integrated modelling and optimisation framework for multi-stage screw compressors utilising Gaussian Process Regression and Bayesian methods. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*. (Status: Peer review in process)
7. **Kumar, A.**, Kovacevic, A., and Chaudhari, A., 2025. Enhancing efficiency in screw compressors through sustainable polyglycol-based lubricants. *MAPAN - Journal of Metrology Society of India*. (Status: Response to reviewer's comments submitted, under "Awaiting Recommendation")

Conference Papers

1. **Kumar, A.**, Kovacevic, A., Ponnusami, S.A., Patil, S., Abdan, S., and Asati, N., 2022, November. On performance optimisation for oil-injected screw compressors using different evolutionary algorithms. *IOP Conference Series: Materials Science and Engineering*, Vol. 1267, No. 1, p. 012021. IOP Publishing.
2. **Kumar, A.**, Kovacevic, A., and Stosic, N., 2024, December. Impact of rotor geometry and fluid injection on screw compressor performance. *IOP Conference Series: Materials Science and Engineering*, Vol. 1322, No. 1, p. 012008. IOP Publishing.
3. **Kumar, A.**, Patil, K., Kulkarni, A., and Patil, S., 2023, September. Investigating alternative rotor materials to increase displacement and efficiency of screw compressor while considering cost and manufacturability. *International Conference on Compressors and their Systems*, pp. 115-125. Cham: Springer Nature Switzerland.
4. **Kumar, A.**, Kovacevic, A., and Anusuya Ponnusami, S., 2024. Optimisation of industrial oil-flooded screw compressors: A comparative analysis of conventional and soft computing approaches. *Herrick Conferences 2024*, July 15-18, 2024, West Lafayette, Indiana, USA.
5. **Kumar, A.**, and Bikramaditya, N., 2024. Advancing sustainability: A comprehensive

- study on energy-efficient screw compressors for biogas applications. *Herrick Conferences 2024*, July 15-18, 2024, West Lafayette, Indiana, USA.
6. **Kumar, A.**, 2023. Structural analysis of screw compressor block using Bayesian machine learning. Presented at the *Indo-German Conference on Computational Mathematics*, Department of Computational and Data Sciences, Indian Institute of Science, Bangalore, 27-30 March 2023.
 7. **Kumar, A.**, Hujare, P., Bhirud, G., Babre, P., Shinde, A., and Kachare, S., 2024. Exploring artificial intelligence applications for advancing screw compressor technology: A comprehensive analysis. Presented at the *International Conference on Advanced Mechanical Engineering and Industrial Management (ICAMEIM)*, Organized by the Department of Mechanical Engineering, Swami Vivekananda Institute of Science Technology, Kolkata, India, 11-13 March 2024.
 8. **Kumar, A.**, Kovacevic, A. and Stosic, N., 2024. Economic assessment of multi-stage screw compressors: A comprehensive lifecycle cost analysis. Presented at the *International Conference on Screw Machines 2024*, TU Dortmund University, Dortmund, Germany, 3-5 September 2024.
 9. **Kumar, A.**, Kovacevic, A., Anusuya Ponnusami, S., and Bikramaditya, N., 2025. Optimisation of economiser port parameters for improved coefficient of performance in an industrial ammonia refrigeration screw compressor. *14th International Conference on Compressors and their Systems*, City St George's, University of London, London, UK, 8-10 September 2025. (Status: Full Paper Submitted for Review)
 10. **Kumar, A.**, Mane, M., and Abbasi, H., 2025. Vibration Analysis and Mitigation in an Oil-Flooded Screw Compressor Using Finite Element Analysis Techniques. *14th International Conference on Compressors and their Systems*, City St George's, University of London, London, UK, 8-10 September 2025. (Status: Full Paper Submitted for Review)
 11. **Kumar, A.**, Cherian, J., and Lu, Y., 2025. Root cause analysis and finite element analysis (FEA) of internal deformation in an industrial oil-flooded air screw compressor to mitigate frequent seizures. *10th International Conference on Compressor and Refrigeration (ICCR)*, Xi'an, China, 9-11 July 2025. (Status: Full Paper Submitted for Review)

Awards

1. **The Best Student Presentation Award:** “Investigating alternative rotor materials to increase displacement and efficiency of screw compressor while considering cost and manufacturability,” 2023, *13th International Conference on Compressors and their Systems*, City St George’s, University of London, UK.
2. **Geoffrey Soar Award:** Recognises a notable paper/presentation made by a Young Member in the field of fluid machinery, awarded by the *Institution of Mechanical Engineers (IMechE)*, UK.
3. **Outstanding Research Award:** Presented at the *Kirloskar Pneumatic Company Limited Research & Development Colloquium* in 2023 & 2024 by the Kirloskar Group.
4. **Chartered Engineer Certification:** Awarded by the *Institution of Mechanical Engineers (IMechE)*, UK. Registration No.: 704765, registered on 30 October 2023. Membership Number: 80582058. The certification recognizes professional competence and commitment to engineering excellence.
5. **IMechE Conference Grant:** Awarded a prestigious travel and research grant of 750 GBP by the *Institution of Mechanical Engineers (IMechE)*, UK, to support participation in the *10th International Conference on Compressor and Refrigeration*, Xi’an, China, July 2025. Application No.: EAC/KDF/OFFER/25/005.

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Appendix A

Modelling Framework: Program Code

This appendix provides the Python program code developed during this study for the modelling framework. The program is designed to facilitate the optimisation of screw compressor parameters using batch file execution and simulation frameworks such as SCORG, Python and GT-SUITE. It employs advanced techniques like Bayesian optimisation, evolutionary algorithms, and repetitive parameter sweeps for comprehensive analysis.

The complete source code for this modelling framework is available on GitHub for reference and future developments:

GitHub Repository: <https://github.com/Krishna281161/Modelling-Framework-for-Multi-Stage-Screw-Compressors>

Program Code

The Python code used in the modelling framework is structured to handle multiple optimisation scenarios, dynamically modify input files, execute simulations, and incorporate different optimisation methodologies. The complete implementation, including the core framework, graphical user interface (GUI), and data processing scripts, is available in the GitHub repository.

Explanation of the Code

The program operates in the following steps:

1. **Batch File Modification:** The `modify_batch_file` function dynamically updates the batch file parameters based on user input or optimisation results.

2. **Batch Execution and Parsing:** The `execute_batch_and_parse` function runs the modified batch file and extracts relevant performance metrics from the output file.
3. **Optimisation Techniques:** The program utilises multiple optimisation methods:
 - **Bayesian Optimisation:** Employs Gaussian Process Regression (GPR) to iteratively refine the search for optimal parameters, reducing computational iterations while ensuring high accuracy.
 - **Evolutionary Algorithm:** Uses a **differential evolution approach** for robust parameter selection, ensuring global convergence and improved search efficiency.
4. **Error Evaluation:** The objective function calculates the absolute error between the simulation results and the target value to assess the model's performance.
5. **Graphical User Interface (GUI) Integration:** A Tkinter-based GUI is provided to allow users to **input parameters, execute batch files, run optimisations, and visualise results interactively.**

Applications

The program enables users to:

- Optimise key parameters for screw compressor design, including **geometry, profile, and fluid injection properties.**
- Evaluate different optimisation methods and their effectiveness in **multi-stage screw compressor performance analysis.**
- Generate insights into **parameter sensitivity, efficiency trade-offs, and system-level improvements.**

Repository Link for Reference

The complete Python implementation of the modelling framework, including the optimisation scripts, batch execution code, and GUI, can be accessed via the GitHub repository:

[https://github.com/Krishna281161/
Modelling-Framework-for-Multi-Stage-Screw-Compressors](https://github.com/Krishna281161/Modelling-Framework-for-Multi-Stage-Screw-Compressors)

Note

This code is specific to the modelling framework developed in this study and is tailored for screw compressor simulation environments. Users must ensure that all dependencies are installed, file paths are correctly configured, and the batch execution setup is appropriately structured before running the program.

Appendix B

Performance Metrics

This appendix outlines the key performance metrics used throughout the thesis for evaluating and optimizing screw compressors. These metrics provide critical insights into the compressor's efficiency, capacity, and energy consumption and are essential for both single and multi-objective optimization.

B.1 Key performance metrics

The following metrics are central to assessing the performance of screw compressors:

- **Power Consumption (P) [kW]:** The total energy input required to operate the compressor, including mechanical losses (e.g., in seals, bearings, and drag due to oil injection). Minimizing power consumption is essential for achieving cost-effective operation.
- **Volume Flow Rate (Q) [m³/min]:** Indicates the volumetric capacity of the compressor, representing the volume of gas delivered per unit time under suction conditions. This metric directly reflects the compressor's output performance.

$$Q = 60 \cdot \frac{\dot{m}}{\rho_0} \quad [\text{m}^3/\text{min}] \quad (\text{B.1})$$

where:

- $\dot{m}$: Mass flow rate (kg/s)
- ρ_0 : Gas density at suction conditions (kg/m³)
- **Volumetric Efficiency (η_{vol}) [%]:** Represents the compressor's ability to utilize its theoretical capacity. It is defined as the ratio of the actual volume flow rate (Q) to the theoretical volume flow rate ($V_{\text{theoretical}}$):

$$\eta_{vol} = \frac{\dot{V}}{V_{\text{theoretical}}} \cdot 100 \quad [\%] \quad (\text{B.2})$$

- **Adiabatic Efficiency (η_{ad}) [%]:** Measures the thermodynamic efficiency of the compression process by comparing the theoretical adiabatic power (P_a) to the actual power consumed (P). It reflects how close the process is to an ideal adiabatic compression:

$$\eta_{ad} = \frac{P_a}{P} \cdot 100 \quad [\%] \quad (\text{B.3})$$

- **Specific Power Consumption (SPC) [kW/m³/min]:** Quantifies the energy required to compress a unit volume of gas. SPC is a critical indicator of the compressor's energy efficiency and is calculated as:

$$SPC = \frac{P}{Q} \quad [\text{kW/m}^3/\text{min}] \quad (\text{B.4})$$

B.2 Explanation and significance

- **Power Consumption (P):** Minimizing P is critical for reducing operating costs and ensuring the compressor runs efficiently over its lifecycle.
- **Volume Flow Rate (Q):** Q reflects the compressor's capacity to handle gas and determines its suitability for specific applications. Higher Q values indicate greater throughput under given operating conditions.
- **Volumetric Efficiency (η_{vol}):** A higher η_{vol} indicates better utilization of the compressor's theoretical capacity, minimizing losses due to leakage, re-expansion, or mechanical inefficiencies.
- **Adiabatic Efficiency (η_{ad}):** As a measure of thermodynamic efficiency, η_{ad} highlights the energy losses incurred during compression. Maximizing η_{ad} leads to reduced energy consumption and enhanced overall performance.
- **Specific Power Consumption (SPC):** SPC is a comprehensive indicator of compressor efficiency, combining P and Q . A lower SPC value signifies a more energy-efficient compressor, making it a critical parameter for sustainable operation.

B.3 Applications in optimisation and design

These performance metrics are used repetitively throughout this thesis for the following purposes:

- **Evaluating Baseline Performance:** Establishing benchmarks for existing single-stage and multi-stage screw compressors.
- **Comparing Compressor Designs:** Identifying the most efficient configurations under varying operating conditions.
- **Guiding Optimization:** Serving as objectives in optimization algorithms, such as minimizing SPC or maximizing η_{vol} and η_{ad} .
- **Supporting Decision-Making:** Providing actionable insights into trade-offs between performance, cost, and energy efficiency.

By integrating these metrics into the modeling and optimization framework, the thesis ensures a consistent and robust approach to performance evaluation across different compressor designs and operational scenarios.