Physics-Driven Generative Design of Rotor Tip in an Experimental Roots Blower Using ToffeeX

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ABSTRACT

Leakage flow through clearance gaps in positive displacement compressors is a significant source of inefficiency. Our research aims to utilise physics-driven generative topology optimisation embedded within a computational fluid dynamics (CFD) solver to redesign the compressor rotor tip profile, such that, for a specified clearance gap size, leakage flow is reduced. This increases the compressor's overall volumetric efficiency and reduces its energy consumption. In this feature paper, we present a physics-based generative design workflow, validate the base leakage flow model using particle image velocimetry test data, and, for a given set of operating conditions, apply the topology optimisation algorithm using the ToffeeX cloud-native CFD solver. The resulting shapes that have evolved through this optimisation process are novel and emphasise that governing flow physics can yield designs beyond engineering intuition. The computational results are presented as an analysis of the gas leakage velocity profile, pressure distribution, pressure drop increment, and overall efficiency gains of our new design.

Keywords: shape optimisation; multiphysics topology technique; CFD; PIV

1. Introduction

Rotary positive displacement machines consist of a rotor, the rotating component, and a casing that serves as the stationary part, enclosing the rotor. Compression happens within sealed chambers as the rotor rotates. A finite volume of air becomes trapped when the lobe passes over the blower inlet and is carried around the chamber by the lobes. As the rotor lobes turn, internal pressure rises upstream of the blower outlet, creating a pressure difference between the discharge and suction sides. This causes air to flow back through the design clearances. For an oil-free machine, such as a roots blower, operation and reliability depend on optimal clearance gaps. These gaps can potentially enhance overall reliability and efficiency. Studies have focused on optimising tip shapes using CFD and practical experience to increase efficiency. Often, optimisation is carried out through trial and error, involving experimental, practical, and numerical challenges. To enable quicker design improvements, engineers and researchers seek more effective optimisation techniques for numerical simulations.

The optimisation of aerodynamic machine designs initially focused on aerospace components. Carlson & Middleton [1] explored this area through airfoil profiles to minimise drag. The first use of topology optimisation in this field dates back to the 1980s, with contributions by Lavrov [2], Glowinski [3] and Goodman [4]. Early research predominantly addressed structural issues and drew on the insights of Bendsoe and Kikuchi [5]. Recently, the scope of optimisation has broadened to include various scientific fields. Topology optimisation is now applied to aerodynamic and electromagnetic problems and has been extended to fluid-thermal systems that involve the Navier-Stokes equations and the convection-conduction equations. For instance, Dede [6] used this technique to optimise power dissipation and average temperature in a heated domain. Yoon [7] examined 2D topology Optimisation with external coolant for cooling a hot plate and extended it to a microchannel system. Matsumori [8] enhanced this method by incorporating a conjugate heat-transfer approach that accounts for both fluid and solid phases. Koga [9] later adapted this technique to a uniformly heated 3D medium to develop a heat sink device. Kyle [10] performed optimisation using an adjoint formulation on unstructured grids, thereby calculating sensitivities of the objective with respect to design variables. Biancolini and Cella [11] employed a Radial Basis Function (RBF) morphing method for coupled CFD–CSM aeroelastic analyses and subsequently applied it to RBF-based mesh smoothing, as reported in Biancolini [12]. The RBF morph was integrated into the Fluent solver to deform meshes while preserving quality. Lombardi [13] demonstrated that RBFs effectively manage in-grid interpolation and mesh motion in FSI simulations. Papoutsis-Kiachagias [14] highlighted the importance of advanced optimisation techniques, especially continuous adjoints and RBF morphing, in efficient automotive aerodynamic design. Porziani [15] developed an automated shape optimisation method that was successfully applied at an industrial scale to accelerate product development. Porziani [16] introduced a bio-inspired algorithm that evolves shapes by gradually modifying geometry in response to specific objectives and constraints. Later, Stefano [17] proposed an optimisation framework that combines mesh morphing with surface sculpting, involving iterative shape modification, simulation, and optimisation.

The analysis of three-dimensional Topology Optimisation (TO) methods for heat transfer in fluid domains and conjugate heat transfer phenomena has been successfully completed. In the conjugate heat transfer problem, the convection-conduction equation was combined with the moving-asymptotes method, as described by Marck [18]. This study involved injecting coolant flow at the inlet of a two-dimensional domain, which was then expelled through the outlet in a uniformly heated domain, with heat diffusing directly from the domain walls. Similar approaches have been used by Pietropaoli [19], who applied a steepest-descent gradient method for comparable problems. Later, they adapted their model to a three-dimensional square duct, focusing on optimising heat transfer while minimising stagnation-pressure loss in the coolant flow. This optimisation was carried out using Toffee, a proprietary tool based on the adjoint optimisation method described by Pietropaoli [19]. Yaji K [20] implemented a topology optimisation method for a coupled thermal–fluid problem using level set boundary expressions.

Industries and researchers across various sectors actively pursue shape optimisation to accelerate the design process. They typically use available software tools to create new shapes through optimisation techniques. However, researchers in compressor technology have shown less interest in shape optimisation with current predictive technologies. Recently, Neeraj [21] applied shape optimisation using the Fluent adjoint solver, combined with RBF morph integration, to improve the tip profile. They also employed Fluent Sculpting, an automated optimisation tool, to demonstrate its effectiveness, noting that mesh quality was maintained during the process. This study aims to leverage ToffeeX's capabilities to develop an improved tip design that reduces leakage flow. The base geometry was simplified compared with the more complex version, and Neeraj [22-23] performed a full transient simulation.

2. Methodology

To optimise shape, various methods are used across industries to enhance machine performance. Recently, industry professionals and researchers have evaluated numerous software options to predict the evolving shapes of machines and their components. Some well-established approaches include the Adjoint method, its integration with RBF morphing techniques, and Thermo-Fluid Optimisation from ToffeeX. ToffeeX is a generative engineering design software used for optimising thermofluidic components and systems. The goal is to assess the ToffeeX software's capacity for positive-displacement machines.

To measure surface temperatures and obtain spatial and temporal temperature fields, Infrared Thermography is a well-known experimental method. Factors such as reflections through clear windows, window types, and approximations of local emissivity variations can influence the measurements. The principle behind infrared thermography is that an object at a temperature above absolute zero emits infrared radiation. Therefore, to obtain the temperature, the radiation intensity can be measured in a test. The Image shown in the figure. 1(a) is an assembly of an IR 8300hp camera that has a specific spectral range of from 2 to 5.7 µm and a temperature range from -40 to 1500 °C. Figure 1(b) is the root blower CAD model displaying the measurement plane, gap, and tip dimensions. To measure the lobe surface temperature during machine operation, the LabVIEW program was configured to trigger the camera using the shaft encoder signal, and phase-locked data acquisition was used to capture data.

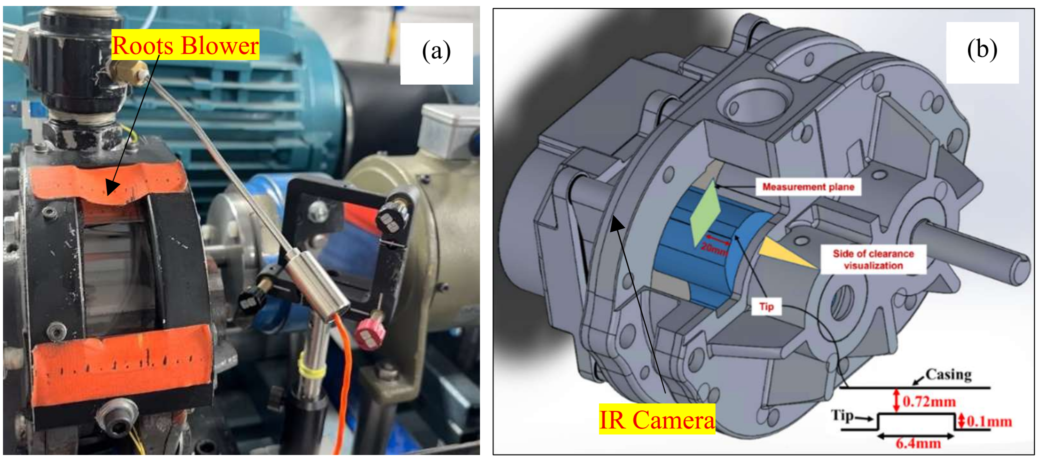

Figure 1. Infrared Thermography – a) Experimental Roots blower; b) Tip Gap.

2.1. CFD Model Validation

The basic fluid flow phenomena were initially obtained using a conventional CFD method implemented in ToffeeX, which solves the mass, momentum, and energy equations. The ideal gas is employed as the working medium. It is regarded as an ideal gas, meaning its density depends only on temperature and pressure. It has the density of an ideal gas, a specific heat of 1005.0 J/(kg · K), a thermal conductivity of 0.0262 W/(m · K), and a viscosity of 1.831×10^{-5} kg/(m · s).

2.2. Tip Gap Optimization Using ToffeeX Solver

ToffeeX is a generative design tool powered by a combination of physics-based simulation and proprietary optimisation algorithms. Toffee is an acronym for **T**opology **O**ptimization **f**or **F**luids **E**ngineering. To enhance performance, the Topology Optimisation method is employed to determine the optimal material layout within a specified design space, accounting for specific boundary conditions and constraints. In topology optimisation, an 'objective function' is defined. This is a mathematical function that analyses the solid field within the design domain (along with other variables that may depend on it) and yields a single value. The optimiser then seeks to find the distribution of solidity that minimises the objective function.
A design domain **Ω**, as shown in Figure 2, is the spatial area where the solution is desired. A set of state variables, x, depends on pressure p, velocity vector v, and temperature T. In this case, we can express the objective function as a weighted sum of two objectives, with weights $\omega 1$ and $\omega 2$ that determine the relative importance of each, as shown in Equation 1. In cases where the objective function F needs to minimise the temperature T and the total pressure dissipation P_o, Equation 1 can be simplified to Equation 2, where F1 is given by Equation 3 for temperature and F2 is given by Equation 4 for total pressure dissipation. To optimise multiple objectives simultaneously, we can finally express the objective function as in Equation 5.

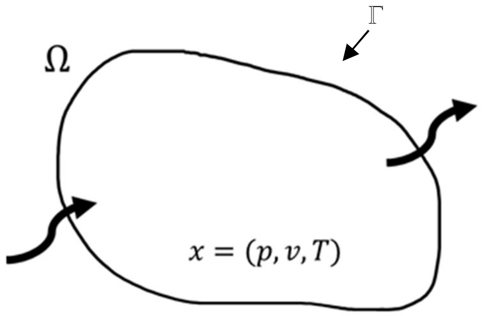

Figure 2. Arbitrary design domain **Ω** with boundary Γ.

$$F = \omega_1 F_1 + \omega_2 F_2 + \omega_3 F_{3t} \dots\dots\dots + \omega_n F_n \quad (1)$$
$$F = \omega_1 F_1 + \omega_2 F_2 \quad (2)$$
$$F_1 = \int_{\Omega} T \, d\Omega \quad (3)$$
$$F_2 = \int_{\Gamma} (P_0) u \cdot \hat{n} \, d\Gamma \quad (4)$$
$$\min_{x,\gamma} F = \omega_1 \int_{\Omega} T \, d\Omega + \omega_2 \int_{\Gamma} (P_0) u \cdot \hat{n} \, d\Gamma \quad (5)$$

If we are simulating fluid flow, the velocity and pressure fields used to define the objective function must satisfy the Navier-Stokes (N-S) equations. If we are simulating heat transfer in a solid, then the temperature must satisfy the heat diffusion equation. For the adjoint optimisation in flow problems, a Lagrangian approach is employed to solve the minimisation problem, as discussed by Qian et al. (2016) and Dilgen et al. (2018). In general formulation, the minimisation of the objective function F (x, γ), where γ is the design variable, is subjected to R(x,γ) = 0. R is the set of constraints, and x represents the set of state variables, such as p, u and T. The final Navier-Stokes and Energy equations are given by Equations (6)-(7) and (8), respectively, for solving fluid-flow adjoint optimisation problems. The details of this formulation can be found in the study by Pietropaoli et al. (2017).

$$R_p = \nabla \cdot u \quad (6)$$
$$R_u = \rho(u \cdot \nabla)u + \nabla p - \mu \Delta u - \alpha u \quad (7)$$
$$R_T = c\rho u \cdot \nabla T - \nabla \cdot (k \nabla T) \quad (8)$$

Figure 3 presents the flowchart of the fluid Topological optimisation process. In this process, the basic flow is first solved after grid generation and boundary-condition specification, with the remaining design parameters. Upon topological optimisation, the design is updated. This process is iterated until convergence.

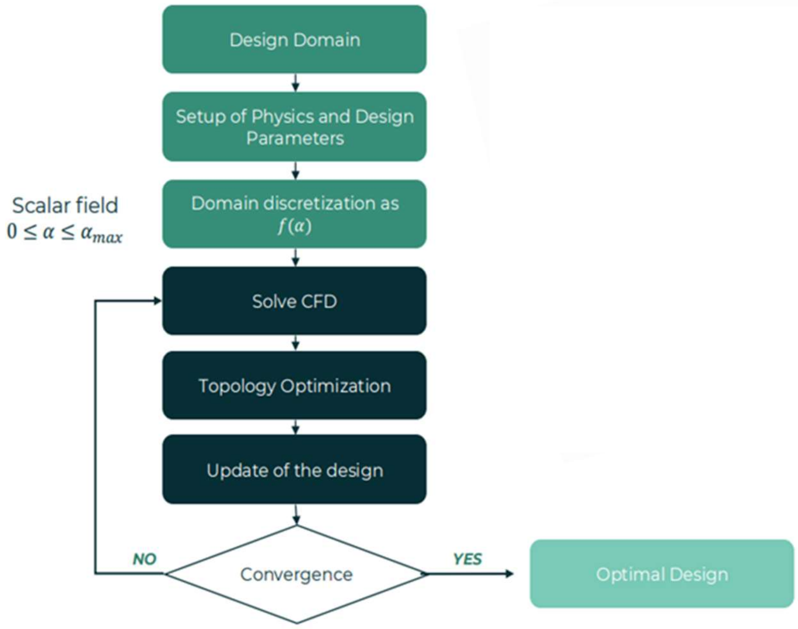

Figure 3. ToffeeX Calculation Flow Chart.

3. Computational Domain & Setup

The computational domain is shown in Figure 4 below, representing a simple stepped-tip geometry, as outlined by Neeraj et al. [21-23]. This model simplifies the original geometry. In this study, the domain is reduced to a 2D representation by considering only the thickness in one direction. The initial Computational Fluid Dynamics (CFD) simulation listed in Table 1 runs under steady-state conditions. The model uses the rotor tip as a wall boundary. The setup closely follows that of Neeraj [21], with a z-thickness of 5 mm. The inlet and outlet boundary conditions are fixed-pressure boundary conditions.

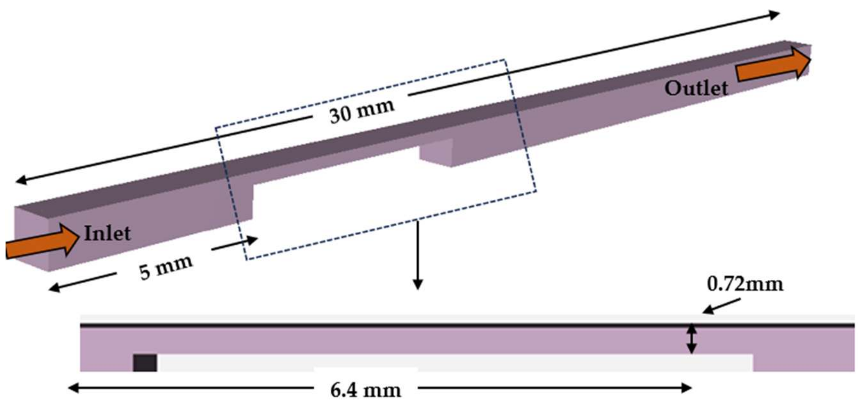

Figure 4. Base-Computational domain and Boundary Conditions (Extracted from Tip – Figure 1).

Table 1. Base CFD Solver Set-up

Items	Specification	Items	Specification
Solver	Pressure based	**Spatial discretization**	2nd Order upwind
Turbulence	K-ω SST	**Turbulence numeric**	2nd Order upwind
Fluid	Air	**Gradient**	Green-Gauss node

P-V Coupling	Coupled	Flux-type	Rhie-chow: mom-based

Figure 5 is the grid representation of the model and its refinement near the tip area. The mesh is 0.6 um in the vicinity of the Tip, and the rest of the grid level is 30-40 times larger than that of the lowest level. This grid was generated using ToffeeX software, which allowed the creation of a hexahedral-dominant mesh, as seen in Figure 5.

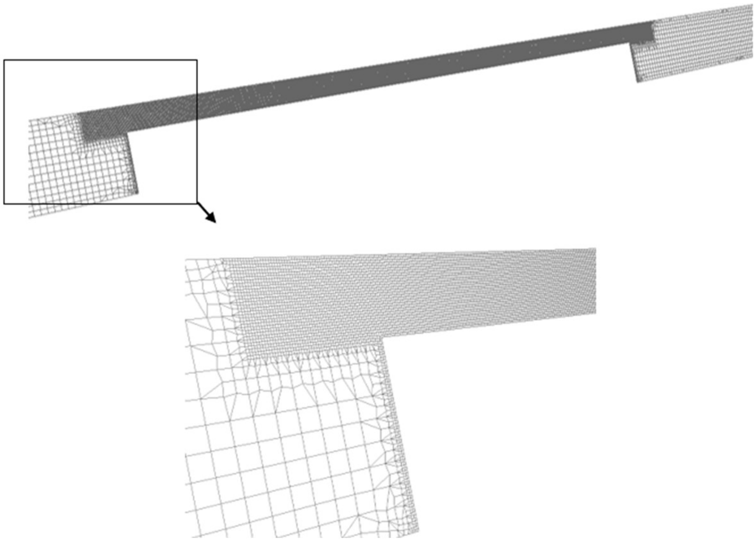

Figure 5. Grid Refinement of the Computational Domain

4. Results & Discussion

4.1. Validation with PIV

The previous section discussed the CFD model and boundary conditions; in this section, a quantitative comparison of velocity profiles is presented to validate the CFD model and setup against PIV results. The velocity profile is compared with that obtained from velocity lines in the clearance gap, as shown in Figure 6, as indicated by Neeraj [23]. The X and Y scales of the comparison graph are based on normalised X & Y positions, defined as the total length of the through and across gap lines, respectively. The indicated X & Y are not Cartesian coordinates.

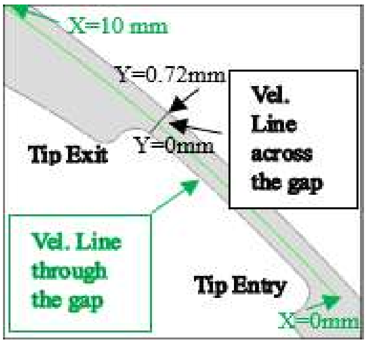

Figure 6. PIV velocity magnitude measurement line description [23].

Figure 7(a) is the velocity profile comparison of PIV and CFD through the clearance gap, which is taken slightly upstream of the tip entry and downstream of exit as shown in Figure 4. The CFD main-gap flow is lower velocity than the PIV flow. A comparison of velocity magnitude deviations from PIV at selected points along the traced line shows approximately 6% deviation, except in the middle, where the deviation is approximately 10%, as shown in Figure 7(b). The discrepancy can be explained by noting that the model is much simpler than the reference geometry and the laboratory test. In this model's geometry, the fillet is missing, and the sharp corners tend to reduce the magnitude of the leakage flow.

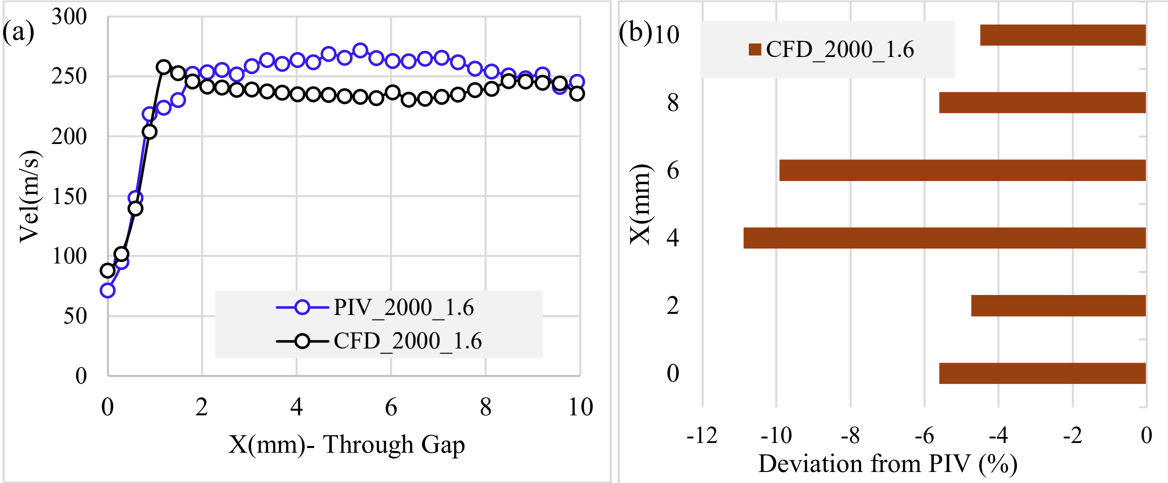

Figure 7. (a) Velocity profile through gap, (b) Velocity magnitude deviation from the PIV measurement.

4.2. Optimisation of Tip Geometry

In this section, the software's optimisation results are presented and discussed across three cases with different inlet velocities. The aim is to change the tip of the lobe to reduce leakage flow. Figure 8 is the comparison of the optimised model result (Figure 8(b)) with the base model (Figure 8(a)). Optimisation has resulted in a filleted tip to reduce leakage flow, thereby forcing the mainstream to broaden. This indicates that the velocity magnitude in the vicinity of the wall has improved, as shown in contour 8(b).

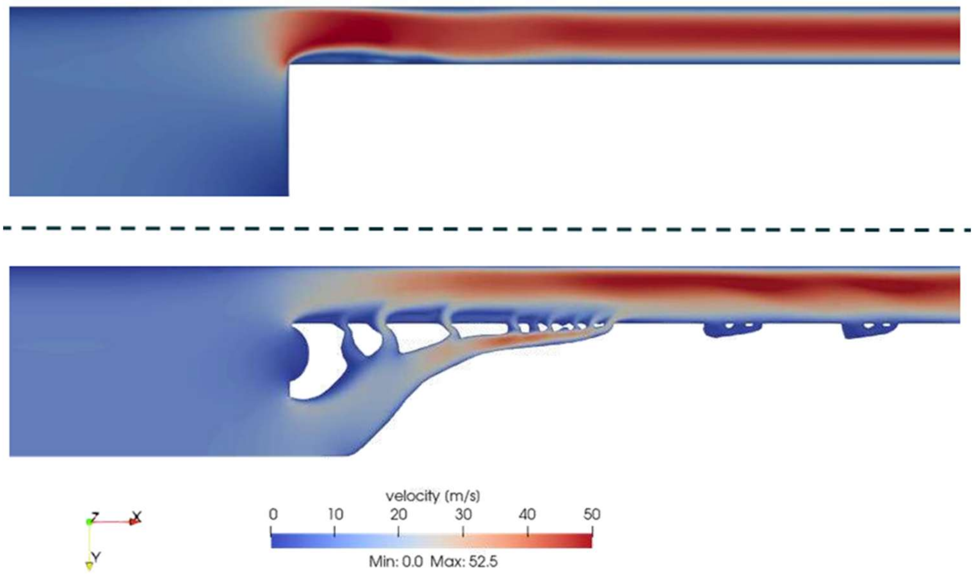

Figure 8. Velocity Contour (a) Base model, (b) Optimised model at Velocity = 10m/s

The comparison of ΔP between the baseline model and the ToffeeX optimised model is shown in Figure 9 (a) & (b). It indicated that the ToffeeX model has a higher ΔP than the Baseline. It was largely improved by a fillet, which increased inlet pressure. This is also indicated in Table 2, where ΔP for the optimised model increases by 250kPa. Table 3 presents a comparison of ΔP across different velocity inlets for the ToffeeX-optimised result and the base-model result.

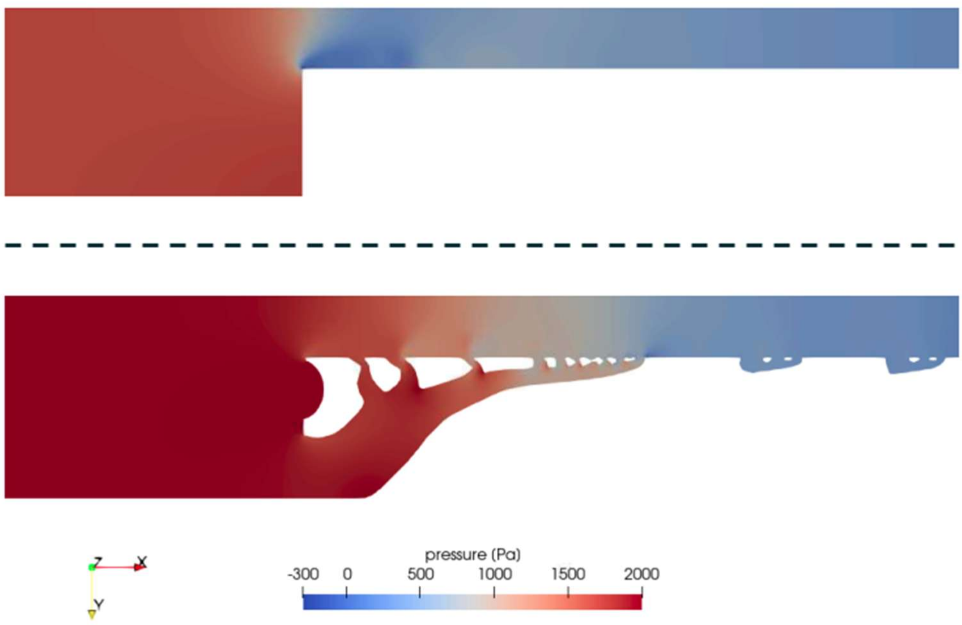

Figure 9. Pressure Contour (a) Base model, (b) Optimised model at Velocity = 10m/s.

Table 2. Comparison of ΔP.

Case	ΔP (kPa)
Baseline	1702
ToffeeX	2044

Table 3. Comparison with Flat tip- Different Flow Rates

Velocity(m/s)	ΔP ToffeeX (kPa)	ΔP Flat (kPa)
10	2.04	1.7
30	17.5	16.8
60	57.9	53.0

A second round of optimisations has been performed, assuming different flow velocities. The optimisation yields different tip topologies under different conditions. This is in line with expectations, as different flow structures will arise and, consequently, the optimiser will propose a different solution to maximise pressure losses. The designer could therefore fine-tune the gap topology based on the design point's profiling. The different topologies are reported in Table 4. The higher flow momentum at 30 m/s or 40 m/s results in greater penetration of the flow into the tip. The structures that reverse the flow direction remain detectable, and this effect is exploited much more as one moves downstream along the tip gap than in the 10 m/s optimisation. Due to higher speed, the blockage effect is maximised to roughly 30% of the tip evolution.

Table 4. Comparison with Flat Tip- Different Flow Rates.

Conditions	Optimised Gap Topology
V=10m/s	
V=30m/s	

V=60m/s	

5. Conclusions

Several numerical analysis studies of rotor profiles have aimed to reduce leakage flow. This is because leakage losses account for a much larger share of overall losses than factors such as mechanical bearing losses or compression pressure ratio mismatch. In machines such as Roots blowers with low internal pressure rise and very high under-compression, the rotor profiles require topology optimisation.

A recent development in computational analysis is Physics-Driven generative design, and it has been implemented in the ToffeeX solver. In this study, the ToffeeX solver was used to design novel rotor profiles that could reduce leakage and improve machine efficiency.

Initially, PIV data from the experimental Roots blower were used to verify the flow field computed by ToffeeX. A mean-line flow deviation of within 10% was recorded using a simplified 2D geometry and averaged representative boundary conditions upstream and downstream of the profile tip, where leakage occurs. The extended analysis performed in this work has proven two concepts:

1. The optimization of the tip at a fixed velocity shows consistent improvements also in off-design conditions imposed via leakage flow velocity.
2. The optimisation of the tip is sensitive to the flow velocity, showing topology variation consistent with higher momentum. Therefore, the designer should select the design speed for optimisation to maximise the benefit of the topologically optimised design.

The use of ToffeeX technology has shown that optimisation can induce a 10-20% pressure drop across the rotor tip thus giving the potential to reduce leakage at the same operating condition. The impact is higher at higher pressure ratio.

In the Future, it will be crucial to apply these methods to the 3D domains of compressors to improve efficiency

Symbol		Abbreviations	
Γ	Boundary of Domain	TO	Topology Optimisation
Ω	Domain	CFD	Computational Fluid Dynamics
F	Objective Function	2D	Two-Dimensional
R	Set of Constraints	3D	Three Dimensional
ω	weights		

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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