Performance evaluation of a novel single-screw compressor and expander design

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Abstract. Single-screw machines have seen significant development and improvement over the last decades and they are currently employed as both compressors and expanders in several applications. The correct functioning of the machine heavily relies on the meshing between the gate rotors and the central rotor which is directly linked to the precision of the manufacturing process to avoid unexpected wear of the tooth profiles. It is well known that the wear of the gate rotor tooth profiles over time is one of the limiting factors with respect to twin-screw machines. To this end, a number of studies have been reported in the literature about improved tooth profiles. For instance, the conventional straight-line profile has been replaced by multi-column tooth flank designs to enlarge the contact surface. However, the manufacturing process is still based on CNC machines with associated challenges.

In a previous study, the authors proposed and modeled a new tooth profile design to overcome the aforementioned limitations. In particular, 3D printing technique was utilized to manufacture the non-conventional tooth design. A geometry model has also been developed to calculate the sealing lines, groove volume curves, and surface areas of the new design.

In this work, a detailed mechanistic model of the single-screw machine is exercised to compare the conventional straight-line profile with the newly proposed tooth profile. Particular emphasis is given to the effect of seal lines on the leakage flows. Furthermore, the design implications of the new tooth profile on internal volume ratio, porting, and displacement are also discussed.

1. Introduction

Single-screw compressors and expanders are widely employed in vapor compression and power generation applications. Since the introduction of single-screw compressors in the early 1960s, the development of single-screw machines progressed due to advancements in the available manufacturing technologies.
Since the working principle of single-screw machines relies on the meshing between a central rotor and two gate rotors (in the PC configuration [1]), the tolerances during the machining process need to be controlled to limit uncertainties on the final groove profile that can yield to a potential rapid wear of the gate rotor tooth flank profile [2].

Over the years, researchers have investigated different meshing profiles to improve the wear resistance and limit leakage flows. For instance, Wu and Feng [3] analyzed the feasibility of employing a multi-column profile (as well as a multi-straight line). Wu et al. [4] introduced a curved flank profile to better distribute the contact forces. Different curve types have been considered including elliptical, hyperbolic, or involute. Li et al. [5] experimentally compared the wear resistance of four tooth profiles, i.e. straight-line, multi-lines, single-column, multi-columns, and found that the single-column profile had the highest wear resistance. Liu et al. [6] introduced a synergy-column design method and its manufacturing process and proved the stable operation of the new profile. A summary of previous studies on multi-column meshing profiles can be found in [7].

With respect to numerical analyses, Wang et al. [8] evaluated the performance improvement of a multi-column profile over a conventional straight-line profile. Results showed that the multi-column profile increased the volumetric efficiency of the compressor over the entire range of operating conditions up to 3.7%. A more in-depth evaluation of a multi-column meshing profile and its effect on leakage flows has been carried out by Wang et al. [7]. The simulation results showed that the multi-column meshing profile was able to reduce both the radial and axial leakage path area of the tooth flank. The column parameters were optimized based on the leakage flow analysis.

In the aforementioned literature, the single-screw profiles have been designed and manufactured by considering multi-axis milling machines. With the advancements of additive manufacturing, limitations on suitable profiles can be overcome and novel single-screw designs can be explored. In particular, in a previous work [9], the authors have proposed a new tooth profile and gate rotor design to improve the control over the meshing process. A prototype of screw rotor and gate rotor was manufactured by employing a 3D printing technique.

The aim of this work is to employ a generalized simulation framework previously developed and validated by the authors to evaluate the performance of the newly designed single-screw meshing pair.
2. Single-screw design

The starting point of designing a single-screw compressor or expander is the definition of the generating profile which also represents the shape of each gate rotor tooth. In most of current applications, straight-line meshing profiles are chosen to generate the grooves of the central screw. The resulting tooth has a characteristic rectangular-like shape, as shown in Figure 1(a). Such tooth design features a meshing plane, an upper flat surface, and a lower surface. Three angles ($\alpha_1$, $\alpha_{11}$, and $\alpha_2$) are usually defined to describe the shape of the tooth and ensure the correct sliding of the meshing plane of the tooth inside the mating screw rotor groove (the complete mathematical formulation can be found in Ziviani et al. [1]).

In the literature, different teeth shapes have been reported and investigated. For examples, Yang and Liang [10] explored the feasibility of adopting conical teeth. A real scale prototype was manufactured with a milling machine, but no performance data was reported. A fan-shaped tooth design was proposed by Murono et al. [11]. Simulation results indicated that the optimal selection of fan angle could lead to an increase in groove volume for a given rotor and gate rotor diameters yielding to possible downsizing of the compressor. However, an excessively large fan angle is likely to cause interference between the gate rotor and the screw groove.

To overcome wearing issues, control over manufacturing process, and explore new design solutions, a new tooth profile and manufacturing technique have been considered by the authors [9]. The tooth design is shown in Figure 1(b). A couple of features can be noted: (i) the meshing plane coincides with the top surface of the gate rotor which facilitates the assembly and alignment; (ii) the tooth profile consists of two straight lines and a circular arch without any discontinuities; (iii) two angles ($\alpha_1$ and $\alpha_2$) are used to control the design of the gate rotor.
supports to facilitate the assembly; (iv) a wear resistance insert can be installed and act as meshing plane; (v) 3D printing has been used to prove the concept design (more details can be found in [9]), and it is shown in Figure 2(a).

![Figure 2](image1.png)

**Figure 2.** (a) View of the 3D printed screw rotor with the new tooth profile; (b) tooth sealing lines of a conventional tooth.

![Figure 3](image2.png)

**Figure 3.** Conventional single-screw expander: (a) Side view; (b) top view.

3. Mechanistic model
In order to evaluate the performance of the new tooth design, a comprehensive mechanistic model of an open-drive single-screw expander that has been previously developed and validated is employed [12]. Since the model has been extensively discussed, only essential assumptions are outlined in the following subsections.

3.1. Non-symmetric approach
The expander model is based on the thermodynamic concept of open-control volume to which mass and energy balance equations are applied. The single-screw expander has been divided into static and dynamic control volumes. The static control volumes describe the inlet shell volumes
that connect the inlet housing inlet port to the two suction ports located on both sides of the rotor as well as the outlet shell volume. The dynamic control volumes represent the grooves of the central rotor. In this model, all the working chambers are considered and therefore a non-symmetric mathematical approach is implemented to have a high-fidelity description of the actual machine. An adaptive RK45 solver is used to integrate the set of differential equations over one working cycle.

For the purpose of this study, particular attention is given to the assumptions concerning the leakage flow models. It is well known that single-screw machines have numerous leakage flow paths. With respect to the meshing between the tooth and the groove, four sealing lines can be identified in a conventional tooth, as shown in Figure 2(b), where the leakage flows are along the groove flanks. In particular, $L_1$ and $L_3$ are associated with the flanks of the tooth, $L_2$ is front of the tooth (gap between front of the tooth and the bottom of the groove), and $L_4$ is the gap between the upper surface of the gate rotor and the housing. In the case of the new tooth profile (see Figure 2(a)), the perimeter of the tooth is a continuous profile. Hence, a single sealing line is considered ($L_1$) to be representative of flanks and front of the tooth. Whereas, $L_4$ still maintains the same definition. Moreover, in a conventional tooth design, besides the leakage flows that are along the groove flanks (see leakage flows through $L_1$ and $L_3$ in Figure 3(a) as examples), blow-holes can be located along the flanks of the tooth due to the design angles of the upper surface ($L_5$ and $L_6$), as illustrated in Figure 3(b), as well as at the corners of the tooth front surface due machining uncertainties of the groove bottom. In this study, all the blow-holes of the conventional design are neglected. In this way, the new tooth design is compared with the best possible conventional design. Furthermore, all the leakage paths ($L_1$ through $L_4$) have a gap size of 10 $\mu$m and length according to the geometry. The choice of meshing clearance gap size is justified by the values reported by Shen et al. [13]. In their study, desired meshing clearance gaps are in the order of 20 $\mu$m. In this work, the best case scenario has been selected. In fact, similarly to the blow-holes, such tight gap sizes represent a high accurate manufacturing process. The leakage flows have been modeled with an isentropic flow model with a flow coefficient of 0.8.

3.2. Overall energy balance
The expander model is closed with an overall energy balance to account for the different thermal interactions inside the machine. The details of the multi-lumped thermal network model can be found in [14]. The overall energy balance of the expander that must be satisfied is given by,

$$\overline{W}_{\text{exp,shaft}} = \dot{m}_{\text{wf}} \left(h_{\text{su}} - h_{\text{ex}}\right) - \sum_i \dot{Q}_i (T_{\text{amb}})$$

where $\overline{W}_{\text{exp,shaft}}$ is the average shaft power over one working cycle, $\dot{m}_{\text{wf}}$ is the working fluid mass flow rate, $h_{\text{su}}$ and $h_{\text{ex}}$ are the suction and discharge specific enthalpies, and $\dot{Q}_i (T_{\text{amb}})$ represents the $i$th heat transfer loss through the housing and is expressed as a function of a thermal resistance $R_{i,\text{amb}}$ [14].

3.3. Performance calculations
A detailed geometry model based on multi-polygon approach is used to compute the volume variation of the working chambers. At each rotation angle and for each tooth engaged, the area, $A_i$, and the position of its centroid ($c_z, c_r$) with respect to the screw rotor rotation axis are determined, and the volume of the groove is obtained as:

$$V(\theta) = \sum_i c_r A_i \Delta \theta$$
Table 1. Single-screw expander reference geometric parameters [15].

| Parameter                      | Units       | Value  |
|-------------------------------|-------------|--------|
| Theoretical displacement      | cm³/rev     | 109    |
| Expander volume ratio         | -           | 5.5    |
| Screw rotor grooves, z_{sr}   | -           | 6      |
| Gate rotor teeth, z_{sw}      | -           | 11     |
| Screw rotor diameter, D_{sr}  | m           | 0.122  |
| Center distance, d_{sr,sw}    | m           | 0.796  D_{sr} |
| Rotor length, L_{rotor}       | m           | 0.112  |
| Tooth width, w_{tooth}        | m           | 0.01835|

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where \( c_z, c_r \) are the coordinates of the centroid along and perpendicular to the screw rotor rotation axis, respectively, and \( \theta \) is the screw rotor crank angle. The polygon approach allows to compute also the sealing lines and groove surface [1].

The volumetric performance of the single-screw expander are expressed in terms of filling factor, which is defined as:

\[
\varphi_{FF} = \frac{\dot{m}_{wf}}{\rho_{su} \dot{V}_{disp,th}} 
\]

where the theoretical displacement rate is calculated as:

\[
\dot{V}_{disp,th} = \frac{2V_{g,1}z_{sr}N_{sr}}{60} 
\]

where \( V_{g,1} \) is the groove volume at suction closure, \( z_{sr} \) is the number of grooves, and \( N_{sr} \) is the rotational speed of the screw rotor.

The overall isentropic efficiency is defined as:

\[
\eta_{is,oa} = \frac{\dot{W}_{exp,shaft}}{\dot{W}_{exp,is}} 
\]

4. Results and discussion

The mechanistic model is utilized to evaluate the new tooth design with particular focus on the leakage flows around the meshing profile. To this end, a single-screw expander reference geometry must be selected to carry on the modeling of the new design to have a fair comparison. Once the new single-screw design is defined, the model is exercised under different operating conditions.

4.1. Expander geometries

An open-drive single-screw expander for organic Rankine cycle applications has been selected to be the reference geometry of this study. The machine has been previously tested and modeled by the authors [15]. The main geometric parameters are listed in Table 1.

In order to conduct a comparison between the conventional tooth and the new design, the main dimensions of the meshing pair have been kept constant. In particular, the screw rotors have the same diameter and length and the gate rotors have same outer diameter and degree of penetration into the groove. The width and length of the teeth have been kept constant and the new design features a circular tip profile. A detailed geometric model has been employed to generate the conventional and new single-screw designs, which are shown in Figure 4(a) and
Figure 4. (a) Conventional single-screw design; (b) novel single-screw design.

Figure 4(b), respectively. To be noted is that the conventional design presents an end rotor chamfer that determines the beginning of the discharge process if operated as an expander (suction closure of operated as a compressor). The new tooth design yields to a different end rotor profile that does not require such chamfer, as reported in [9]. Moreover, the suction port in the conventional single-screw expander design has a triangular shape [1] to match the shape of the end of the groove. In the new design, the port has been modified to have a rounded shape to reflect the end groove shape determined by the circular tooth profile.

As a result of the modeling, the new single-screw design has a slightly lower internal volume ratio ($\approx 5.3$) and larger displacement total displacement ($\approx 112 \text{ cm}^3/\text{rev}$). The geometry model with polygon clipping algorithm calculates the length of the sealing lines throughout one rotation of the screw rotor. Figure 5(a) and Figure 5(b) show the instantaneous tooth sealing lines for the conventional tooth and the new tooth design, respectively. As previously mentioned, the conventional tooth design has three edges ($L1$, $L2$, $L3$) and consequently three major sealing
Figure 5. Tooth sealing lines and perimeter as a function of screw rotor crank angle: (a) conventional tooth design; (b) new tooth design.

Table 2. Expander working conditions.

| Parameter               | Value           |
|-------------------------|-----------------|
| Working fluid           | R245fa          |
| Suction temperature, $T_{su}$ | 124.2 °C       |
| Discharge pressure, $p_{ex}$ | 218.8 kPa     |
| Pressure ratio, $r_p$   | 4.5, 6, 8       |
| Rotational speed, $N_{sr}$ | 3000 rpm      |

lines. The fourth sealing line ($L_4$) is the gap between the top surface of the tooth and the housing to allow the rotation of the gate rotor. Whereas, the new tooth design has one continuous sealing line ($L_1$). Around $\theta_{sr} \simeq \pi$, the teeth start disengaging from the grooves, and the sealing lines decrease their length until the teeth is completely outside the meting grooves. As a general qualitative assessment, the total perimeter of the sealing lines of the two designs are comparable, but the conventional tooth does have longer perimeter due to multiple edges constantly engaged.

4.2. Parametric study

A parametric study has been conducted to evaluate the effect of leakage flows on the two single-screw expander designs under different operating conditions. The working fluid of the expander is R245fa and the suction inlet temperature, discharge pressure, and screw rotor rotational speed have been fixed according to the previous experimental campaign [15]. Three different pressure ratios representative of over- and under-expansion operations of the expander have been applied to exercise the model. The operating conditions are summarized in Table 2. In this study, the presence of oil is not considered due high uncertainties on the oil film thicknesses.

In Figure 6(a), a direct comparison between the average leakage flows of the conventional tooth design and the new tooth design at different pressure ratios is shown. The average leakage mass flow rates correspond to a single tooth, since the all the control volumes reaches the same steady-periodic solution. It can be seen that the magnitude of leakage flows through $L_4$ is consistent between the two profiles since the gap sizes are identical, and the total length of that path for both tooth designs is comparable (see $L_4$ in Figure 5(a) and Figure 5(b)). With respect to the sealing lines that are engaged inside the groove, the sum of leakage flows through $L_1$, $L_2$, $L_3$ of the conventional tooth design is slightly lower than the leakage flow through $L_1$ of
the new tooth design. The reason is to be found in the slightly larger displacement of the new expander design. It can also be seen that leakage flow through $L1$ of the conventional design is the highest among the tooth sealing lines and that is consistent with the analysis conducted by Shen et al. [16]. As general comment, the best case scenario has been chosen for the conventional tooth design and the volumetric performance of the two designs are very close to each other. In reality, manufacturing tolerances yield to gap sizes in the order or $30 \mu m - 50 \mu m$ and additional blow-holes with similar dimensions that impact negatively on the volumetric performance of the machine. The key advantage of the new design is the improved control over the meshing line during the manufacturing that could reduce the wear over time, especially if proper lubrication is ensured.

The performance of the expanders is reported in Figure 6(b). In particular, the shaft power output and the total mass flow rate are plotted as a function of the imposed pressure ratios. It can be seen that both mass flow rate and shaft power output increase with the increase of the pressure ratio, which are expected. Due to larger displacement, the new single-screw design delivers high mass flow rates and generates more power under the same operating conditions.

5. Conclusions
In this paper, a new tooth profile design for single-screw machines have been introduced and modeled. The new design aims at reducing common shortcomings of conventional tooth designs in terms of control of manufacturing process, wear, and sizing of the machine. A detailed mechanistic model has been employed to assess the performance of the new tooth design in
comparison with the conventional one. The comparison has been conducted under the most favorable conditions of the conventional tooth, i.e. perfect machining without blow-holes and constant gap sizes. Results showed that the two profiles performed similarly in term of volumetric efficiency within the groove. Leakage flow rates through the sealing lines were comparable. However, if the additional leakage gaps are taken into account, the new tooth profile leads to lower leakage flows. The new expander design showed higher power output due to slightly higher displacement. To further investigate the new tooth profile and its wear over time, an experimental campaign will be conducted to verify the advantages of the continuous tooth sealing lines.

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