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Numerical simulation of labyrinth seals for pulsed compression reactors (PCR)

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Abstract. A sealing system is proposed using labyrinth seals to minimize gas leaks, for which triangular, rectangular, and trapezoidal geometric parameters are evaluated. For each one of the geometries a group of parameters were optimized minimizing the gas leakage, using the multi-objective genetic algorithm (MOGA), updating in each step the geometry employing a user defined Ansys SpaceClaim Python algorithm. For a new set of parameters (height, width, and angle of the shape, space between cavities, and piston length) the script creates the boundary geometry and meshing. The CFD analysis evaluates the gas leakage for the given geometry and constant boundary conditions (10 MPa inlet pressure, 25 m/s piston speed, 40 μm piston/cylinder gap, and ideal methane gas), and uses this data as input to MOGA. The input set values were reduced to manufacturable quantities, so finite or discrete values can be used across the iterations. The analysis of distributed properties such as velocity, temperature, and pression, inside the cavity, showed a steady laminar regime with an energy loss due to entropy increment. The most sensitive parameters are the piston length and height cavity for all shapes. The trapezoidal shape presented the best performance in minimizing the mass flow leakage.

Keywords: Labyrinth seals, pulsed compression reactor, CFD simulation, Ansys Fluent

1 Introduction

Pulsed compression reactor (PCR) have many applications, such as: production of alkenes by dehydrogenation of paraffins; gas and hydrogen synthesis; thermal destruction of impurities that are discharged in industrial process exhaust (air cleaning) and toxic compounds; production of acetylene, nitric oxide, hydrogen cyanide; controlled generation of mono dispersed ceramic, metallic and amorphous nanoparticles by thermal decomposition of appropriate precursors (carbonyl and organometallic compounds, salts, etc.), Kronberg [1].

Many efforts have already been made to develop a commercial chemical reactor based on the principle of pulsed compression. Authors who carried out detailed investigations are Longwell *et al* [2], Kolbanovskiy [3], Morrison & Reimer [4]; however, single shot compression machines are not suitable for industrial applications, Kronberg [1]. On the other hand, many researchers as Von Szeszih [5], Jan & Van Dijck [6], Van Dijck [7], Oberdorfer & Winch [8], Yamamoto *et al* [9], Karim & Moore [10], Karim & Moore [11], Lowther [12], and Dolinsky *et al* [13], tried to use internal combustion engine designs or similar as reactors. However, the commercial applications of internal combustion engines as reactors are limited for a variety of reasons: because it uses oil lubrication, high losses due to cooling (up to 30%), relatively low maximum inlet and outlet pressures, possible sharp decrease in volumetric efficiency with size, inability to continuously adjust the compression ratio as the composition of the reactant's changes, Kronberg [1].

Engineering and reactor design problems for large-scale production of PCRs are thermal control and necessary stabilization for long-term operation, effective start-up methods, gas exchange in chambers (geometry of the chambers, position, size and shape), piston and cylinder materials, and effective lubrication and sealing [1]. The objective is to provide stable and wear-free of the piston and sealing, and to prevent gas leakage through the space between cylinder and piston (gap).

The problem that will be addressed here is the lubrication and sealing, and therefore an effective sealing. Schaller *et al* [14] and Wang *et al* [15] stated that oil-free lubrication carries the gas completely dry and avoids gas contamination due to oil. Also, if PCRs are equipped with a non-contact seal it would have no wear and almost unlimited service life. The distinctive feature of the piston compressor with labyrinth seals is that it does not produce friction between the cylinder-piston, Kläy [16]. So, the method for minimizing leakage, lubrication and sealing is to use a labyrinth seal in the piston, cylinder, or both.

2 PCR labyrinth seal

A labyrinth seal is a structure that consists of multiple cavities where the flow circulates inside them and due to the friction with the walls, the kinetic energy of the fluid is dissipated, thus reducing the leakage flow. The advantages of labyrinth seals are simplicity, robustness, and suitability for high pressures, Schaller *et al* [17]. Instead of piston rings, the labyrinths in the piston are provided with a large number of grooves that produce a labyrinthic sealing effect against the cylinder wall, which is also grooved; the piston moves with enough free space so that there is no contact between the piston and the cylinder wall, Kläy [16].

Graunke & Ronnert [18] showed that the first labyrinth seal equipped compressor was built in 1935. They explained the sealing action of the labyrinth as due to pressure differences from one chamber to another, the throttle point acts as a nozzle for the gas. Part of the pressure energy in the previous chamber is converted into kinetic energy at the nozzle. In the next chamber, the velocity lags almost to zero, and the kinetic energy dissipates in part as heat and in part as vortex energy. By providing a succession of these throttle point and chamber systems, the pressure is reduced from the high level before the piston to the low level after it. The flow process in the labyrinth can be described theoretically by some differential equations as the ideal gas state equation, the continuity equation, the equation of motion or the law of momentum, and the law of conservation of energy.

Most of the research related to labyrinth seals study the rotor-stator system, that is, for rotating elements, and those that study the cylinder-piston system basically focus on the effects of geometric parameters, Wang et al [15]. Cangioli *et al* [19], Cangioli *et al* [20], Hodkinson [21], Milne-Thomson [22], and Vermes [23] explored the labyrinth seal flow calculation method. Currently the main research methods for labyrinth leaks are the analysis of thermodynamic theory, numerical analysis method, leak measurements, flow visualization method. Other studies investigated the mechanism in rotating machines and combined the CFD method, and theoretical analysis to study the flow pattern within the labyrinth seal and analyze the effect of the structural arrangement and the pressure relationship on the sealing efficiency, Wang et al [15].

Encontech B.V. [24] uses a free piston pulsed compression reactor to achieve adiabatic compression. If gas compression is achieved without heat loss, this is accompanied by increases in gas temperature, and if the compression is fast enough, the process approaches an adiabatic one. When using this method, a complete cycle does not exceed 0.01 seconds, the period of time with extreme temperatures and pressures is around 0.001, this short period makes minimal the heat exchange between the gas and the cylinder walls, Glouchenkov *et al* [25]. In this method, a mixture of reactive gases in a tube is compressed by a free piston that moves at a speed of 5-40 m/s, Kronberg [1].

3 Model

The main objective of this study is the parameter's optimization of a PCR labyrinth seal. As seen in Fig. 1, three different geometries will be analyzed, with triangular, rectangular, and trapezoidal shapes. The parameters needed to define each shape are the piston diameter, piston length, gap between piston and cylinder, cavity length, cavity depth, cavity angle, initial free length, and distance between cavities. The piston diameter and gap are considered constants through the present work and stated as 60 mm and 40 μm, respectively. The remaining parameters can vary within the limit values given in Tab. 1.

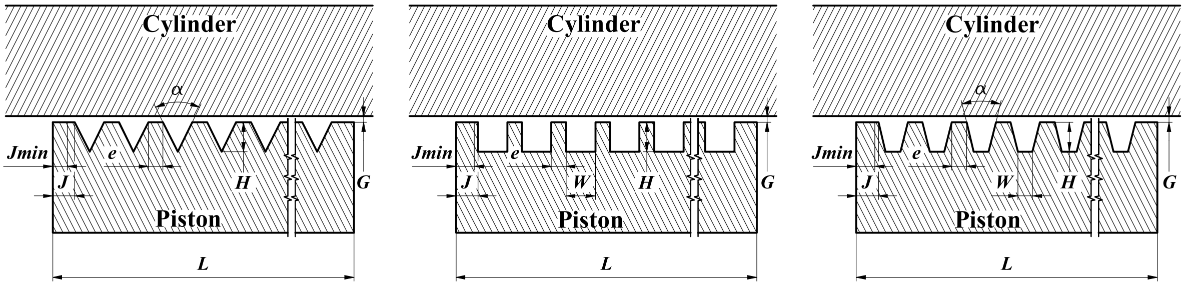

Figure 1. Geometry definition for triangular, rectangular, and trapezoidal shapes

Table 1. Constant and limit values for given cavity geometry

Piston diameter* ***d*** [mm]	Gap between piston and cylinder* ***G*** [μm]	Piston length ***L*** [mm]	Cavity length ***W*** [μm]	Cavity depth ***H*** [mm]	Cavity angle ***α*** [°]	Initial free length J_{min} [mm]	Distance between cavities ***e*** [mm]
60	40	30 - 150	0.5-5.0	0.5-5.0	30 - 75	2.0	1.0 – 5.0

* Constant values

The generation of the parametric geometries is crucial to carry out the optimization process. For this, it was decided to automate this process using scripts, because it reduces the time used to modify the geometry. The CAD program Ansys SpaceClaim was chosen for this study because it presents a user-friendly development environment, a script in the Python programming language will be developed for each of the shapes of the labyrinth seals. Each of the parameters is defined within the limits shown in Table 1, which will for manufacturable values.

The geometries returned by the scripts are two-dimensional geometries that represent the fluid domain. It was decided to use two-dimensional geometries for the study, because it is expected that the fluid presents an axisymmetric behavior. This behavior reduces the computational resources, compared to a three-dimensional study.

Meshing represents an important aspect within the study since an inadequate meshing can cause convergence problems during the simulation process. The criteria to generate the meshing were: aspect ratio $AR \approx 1$; orthogonal quality $OQ \approx 1$, and dimensionless wall distance $y^{+} \approx$ 30-300. The meshing was carried out using triangular and quadrilateral elements.

Table 2. Ansys Fluent model parameters

Gas model	Turbulence Model	C_2	σ_k	σ_ε
Ideal gas (piecewise-polynomial)	Realizable *k*-*ε*	1.9	1.0	1.2

Table 3. Boundary conditions of the model

Gas	Inlet BC	Outlet BC	Piston speed
Methane, $\mathbf{CH_4}$ (compressible gas)	**10 MPa @**300 K	Atmospheric 0 MPa @300 K	**25 m/s**

Ansys Fluent software was used for the fluid analysis of the three proposed labyrinth seal shapes. Within the software, the simulator type was configured as based on pressure and axisymmetric analysis. The Realizable k-epsilon viscosity model was chosen, as it showed better convergence compared to the other variations of k-epsilon model and k-omega models. Also, the software Theory Guide recommends this model in cases where the flow characteristics includes vortices [26]. Table 2 shows Ansys Fluent´s parameters values for this model. Table 3 shows the boundary conditions. This research project is mainly focused on the compression of methane, whereby methane is used as a compressible gas, inlet gauge static pressure being 10 MPa, outlet gauge pressure 0 MPa (atmospheric), and a piston speed of 25 m/s.

4 Results

For the case of the boundary inlet pressure condition, it was seen that the fluid within the domain exhibited supersonic behavior for the given conditions. It is for this reason that an initial static pressure "Supersonic / Initial Gauge Pressure" was used, with a value of 0.95 times the gauge static pressure of 10MPa. For the definition of the gauge total inlet pressure, eq. (1) was used to define it as a function of the inlet static pressure. The expression is based on the solution shown by Ansys Customer Portal [27] for this type of situation, the coefficient a was set as 1. In addition, the "Prevent Reverse Flow" condition was placed at the input. The number of iterations for each simulation was limited to 1500 iterations, which shows that for this number the convergence was acceptable.

$$P_o = P_o(n-1) - a\big(P_s(n-1) - P_{s\,target}\big) \quad (1)$$

where: n, iteration
P_o, gauge total pressure
a, coefficient
P_s, gauge static pressure
$P_{s\,target}$, target gauge static pressure

A parameter correlation study was carried out. This study was based on the leakage mass flow as output parameter. The Spearman method was chosen, with a range of 50 samples per cavity shape. Each of the samples were determined based on the limits of each geometric parameter. Each parameters sensitivity was obtained, and their values are shown in Fig. 2. For all shapes, the piston length is the most sensitive parameter, and the other parameters differ in dependence on the shape. The quadratic regression's coefficient of determination R^2 of leakage mass flow obtained was 0.97 in triangular, 0.78 in rectangular and 0.79 in trapezoidal shape.

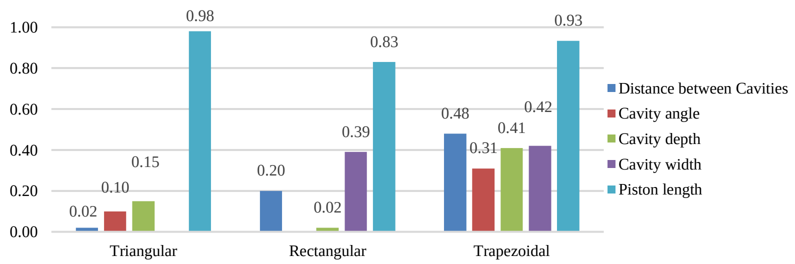

Figure 2. Parameter´s sensitivity

To determine an approximate leakage mass flow mathematical model, with the geometric parameters as input variables, a surface fitting was carried out. The Ansys Response Surface Type's Genetic Aggregation method was used, where the previous 50 samples, used in the parameter correlation, were taken as a basis. Figure 3 shows the mass flow leakage surface for the piston length and space between cavities as input variables, respectively, for the three shapes. These surfaces were obtained by surface fitting, as stated previously, with a Coefficient of Determination R^2 of Learning Points (quality of the interpolation) and Cross-Validation on Learning Points (stability or reliability of the response surface) on Learning Points, 1-1 respectively in triangular, 1-0.98 in rectangular and 1-0.99 in trapezoidal shape.

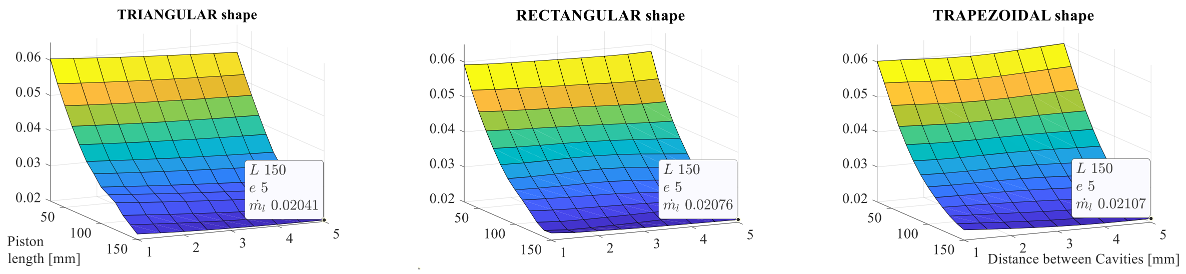

Figure 3. Mass flow leakage for optimal triangular, rectangular, and trapezoidal shape

The flow streamlines for the three shapes are plotted in Fig. 4. For the triangular one, the primary vortex generates minor secondary ones near the vertex. In all cases is seen a centered main vortex displaced slightly to the flow direction. Turbulence is generated at the shape inlet and outlet, caused by the abrupted gas expansion and compression, respectively. The reduction in kinetic energy is greatly influenced by piston speed. The velocity profile is more distorted at the trapezoidal shape, causing higher friction at the walls and therefore higher pressure drop than the other two cavities. Also is seen at the velocity profile along the gap, that the velocity is zero at the cylinder wall (which remains static) and negative at the piston wall (which moves opposite the flow).

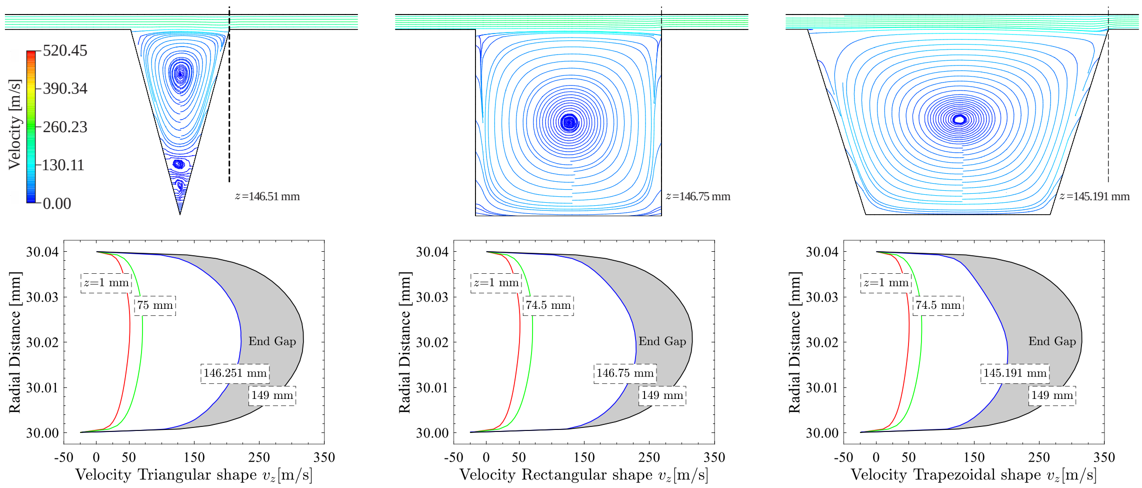

Figure 4. Flow streamline and velocity profile for optimal triangular, rectangular, and trapezoidal shape

Figure 5 shows the pressure drop along the piston, as well as the increase in the kinetic energy of turbulence. As shown in the figure the pressure drop begins to increase from 90 mm and represents approximately the 59.86% of the total pressure drop, in the four cases that includes the 3 shapes of labyrinth seals proposed and the case in which there is no labyrinth seals. Along the turbulence kinetic energy curve there are some peaks for each case, these peaks represent the effect it has on the fluid at the entrance to each cavity. In the same way, can be seen peaks of less size over the pressure curve. It is clearly seen in the figure that the curves of the case without labyrinth seals do not present these peaks, so this confirms the effect that the cavities have on the fluid.

To explain the behavior of the cavity, the distribution profile of temperature (TD), pressure (PD), total energy (TED) and turbulent kinetic energy (TKED), and entropy (ED) were calculated. What occurs in TED is a decrease in the energy in the cavity in relation to the energy in the gap, being less in the center and increased towards the extremes. This means that there is energy consumption, which is what it seeks, which will be responsible for the rotation of the fluid within the cavity. To explain this, we see that the PD and TD follow approximately the same distribution. A decrease in temperature and pressure leads to an increase and decrease in entropy, respectively. As the pressure variation is greater, then there is a liquid increase in entropy that is transformed into irreversibility (heat), which is precisely what is seen in the ED.

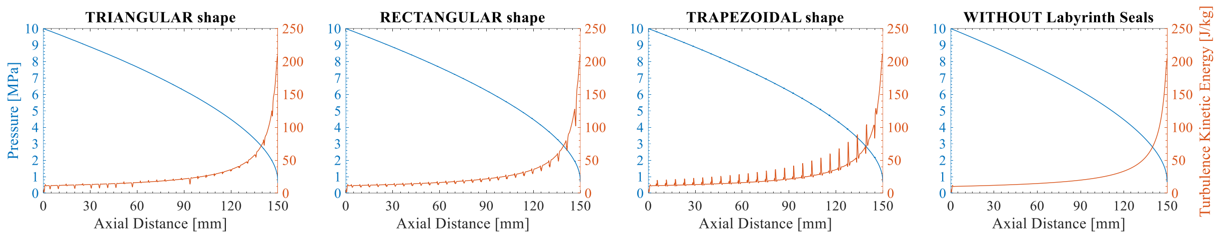

Figure 5. Drop pressure and increase Turbulence kinetic energy along the piston

For the optimization of the geometric parameters minimizing the gas leakage, the multi-objective genetic algorithm MOGA method was used. The maximum allowable pareto percetage MAPP and converge stability percetage CSP conditions where setted at 70% the 2%, respectively. The optimization was carried out based on the surface fitting using the ANSYS Design Exploration tool. Three optimization candidates were considered, after which a verification was made, simulating then each of the three candidates. This process was repeated for each of the proposed labyrinth seal shapes, i.e. for triangular, rectangular, and trapezoidal shapes.

The leakage mass flow for the trapezoidal shape is 0.02007 kg/s (1% with respect the smooth piston), which represents the lowest value of all shapes, Tab. 4. Triangular and rectangular shapes have more leakage mass than smooth piston configuration. This behavior has also been observed by Schaller *et al* [17], who studied a hydrogen compressor with rectangular labyrinth shape for pressure differences of up to 1 MPa and 50 μm gap, pointing out a critical gap value below which the smooth or linear seal shape performs better than the caved ones. A better understanding of the gap effect, and the influence on the type of flow regime (laminar / turbulent) is required.

Table 4. Optimal parameter values for given cavity geometry

Parameters	Without Labyrinth Seals	Triangular	Rectangular	Trapezoidal
Distance between cavities, [mm]	-	5	5	5
Cavity angle, [deg.]	-	30	-	35
Cavity length, [mm]	-	-	0.5	0.5
Cavity depth, [mm]	-	0.5	0.5	0.5
Piston Length, [mm]	150	150	150	150
Mass Flow Leakage, [kg/s]	0.02027	0.02049	0.02050	0.02007

5 Conclusions

The simulation and optimization of the labyrinth seal for PCR with triangular, rectangular, and trapezoidal shapes was carried out successfully, for all cases a set of optimal values of geometry parameters was found. For a 60 mm piston length, 40 μm gap and methane gas at 10 MPa as fluid source. The dimension parameters of the shapes were optimized, and the piston length resulted as the most sensitive. Because of this, other cavity parameters as angle, depth, width and spacing were less important, so consequently, results for a smooth cylinder piston presented a similar performance that those caved.

The analysis of distributed properties such as velocity, temperature, and pression, inside the cavity, showed a steady laminar regime with an energy loss due to entropy increment, greater variation (peaks) of TKE and vorticity was observed in the inlet and outlet of cavities. Also, the reduction in kinetic energy is greatly influenced by piston speed. The trapezoidal shape presented the best performance to minimize the mass flow leakage, with a cavity angle of 35 °, cavity depth of 0.5 mm, distance between cavities of 5 mm and a piston length of 150 mm, on the other hand the that least performance presented was the rectangular shape.

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