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NUMERICAL STUDY OF FLOW INSIDE SUPERSONIC SEPARATORS

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Abstract. *The aim of this project is to study the physics of the phenomena occurring inside a CO_2 /CH_4 supersonic separator by means of 3D numerical simulations focusing on the different options for design and their role on some important flow parameters, like shock wave position and swirl intensity. Besides that, we also implemented a genetic algorithm to optimize the gas separation with respect to two objectives: increase the swirl intensity on the collector section, and its cooling power*

Keywords: CFD, Supersonic Separator, Natural gas, Optimization, Genetic Algorithm.

1. INTRODUCTION

This aim of this project is to explore a novel technology to separate natural gas components, in special water vapour, acid gases like CO_2 and H_2S, and heavy hydrocarbons, known as C_{3+}, in order to comply with technical specifications of transportation into gas pipes, and specifications of heat power. The first is explained by the risk of some fractions condensate, therefore leading to pipe corrosion and formation of hydrates. And the second is justified by the presence of fractions with low calorific value.

The operating principle of this technology is illustrated in figure 1, and it is based on the combination of the cooling properties of a converging-diverging nozzle with the principles of centrifugal separation (Haghighi, *et al.*, 2016). The fluid acceleration to transonic speeds lower the gases temperature, and the swirl leads the higher density fractions (in this case the condensed gases) toward the borders. This technology has some advantages regarding the other options available on market such as the less energy wasted due to the less power required to compress the condensed fraction, less maintenance requirements, reduced size and absence of chemical reactions and of rotating parts.

The main manufacturers of this device nowadays are Engo 3S (figure 1), which is a russian company, and Twister BV (figure 2), a joint venture between Shell and Beacon Group. Both enterprises provide solutions to the separation process, however their products have some distinctions that arise due to the central body design. While Engo 3S' central body has just the role to induce swirl, Twister BV's product has a complex central body, whose function is, besides swirling induction, to define the nozzle profile, which impacts directly to the fluid acceleration. These geometries compose the state of art and the differences among them will reflect on the models designed for this project.

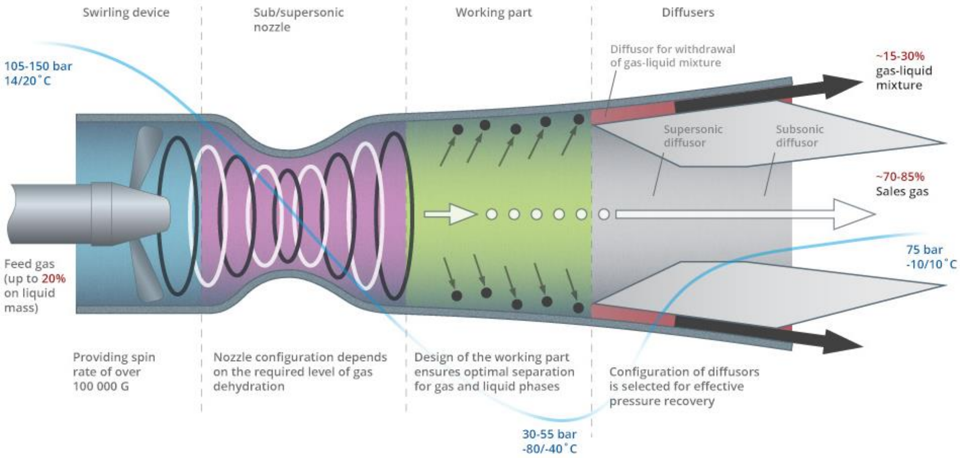

Figure 1 – Supersonic separator scheme (Engo3S, 2017)

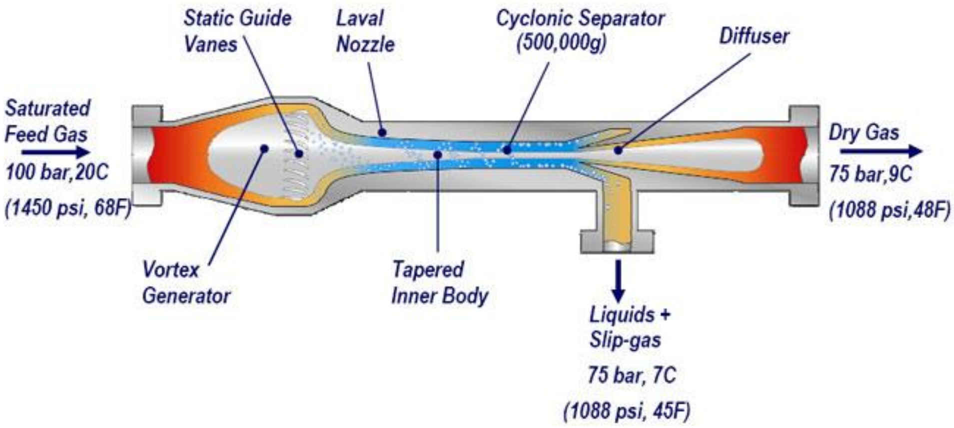

Figure 2. Supersonic Separator Twister Mark II (Twister BV, 2017)

2. MATERIALS AND METHODS

The CFD software and mesh generator employed were respectively ANSYS Fluent and ANSYS Mesh. The mesh grids used for most simulations are unstructured, and the stop criteria for the simulation is set up to a residual below 10^{-4}, except for energy, which is below 10^{-6}. Besides that, aiming to establish interaction between Fluent and the optimization routine, Python language was selected, once it allows the optimization without an explicit function. This means that pre-selected outputs of Fluent calculations can be inputs on the optimization routine cyclically.

Fluent solver was designed to solve the differential equations based on the finite volume method. The transport equations are summarized in equation 1, in which ϕ represents a given specific property, ψ is its diffusion coefficient and S its source term. Table 1 gives the parameters for a single phase flow.

$$\frac{\partial \rho \emptyset_k}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j \emptyset_k - \psi_k \frac{\partial \emptyset_k}{\partial x_j}\right) = S_{\emptyset_k} \tag{1}$$

Table 1. Coefficients for transport equation (Date, 2005; ANSYS, 2016)

Properties	ϕ	ψ	S
Mass	*1*	*0*	*0*
Momentum	u_j	μ	$-\frac{\partial p}{\partial x_i} + \rho B_i + S_{ui}$
Energy	T	$\frac{k}{c_p}$	$\frac{Q'''}{c_p}$
k	K	ψ_k	$G_k - Y_k + S_k$
ω	Ω	ψ_ω	$G_\omega - Y_\omega + S_\omega$

2.1 Fluent set up

The boundary conditions are set up according to the values proposed in Arina (2004 The pressure-based solver of Fluent was used with the coupled option for the pressure-velocity coupling algorithm, which solves simultaneously the momentum and pressure based continuity equations (ANSYS, 2016). The turbulence model applied for the swirling cases is the k-ω SST, which, after a series of tests has shown to be the most accurate among the RANS two-equation models available in the Fluent code. In addition, according to (ANSYS, 2016), k-w SST is recommended for flows with adverse pressure gradient, airfoils and shock-waves.

2.2 Optimization routine development

Among several optimization algorithms available, genetic algorithm was chosen due to its efficiency when dealing with highly non-linear problems. According to (Sheppard, 2016), the algorithm consists in a computer program capable of recognize an individual as an object to which both a chromosome and a fitness value are attributed. Then, a set of individuals compose the initial population, so that the program can select the best individuals among the generation. Before arranging the next population, cross over and mutation processes are done to increase variability, and new generations are originated until the stop condition is reached. Figure 3 sums up the entire algorithm processes.

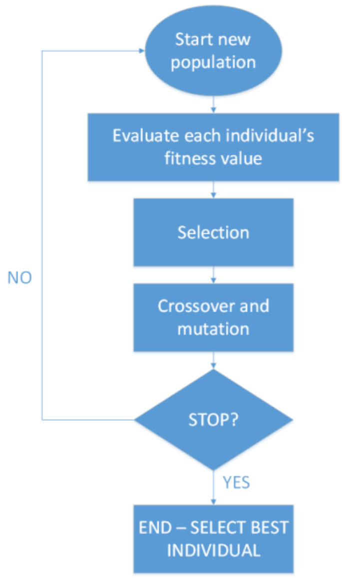

Figure 3. Genetic Algorithm Scheme

Multi-objective routines are employed when more than one objective is relevant to be optimized. For this project the Pareto-optimal approach will be used. According to (Konak *et al.*, 2006), the method aims to find the Pareto border, the set of solutions in which no individual is dominated. The concept of domination is purely mathematical and can be summed up on the following statement: X_1 dominates X_2 only if both conditions of table 2 are valid.

Table 2. Conditions for dominance (Konak, *et al.*, 2016)

	Statement
Condition 1	For every i, $f_i(x_1) \geq f_i(x_2)$
Condition 2	Exist an i for which $f_i(x_1) > f_i(x_2)$

3. RESULTS AND DISCUSSION

Overall, two nozzles and three central body models were studied, as shown in figures 4 and 5. we will refer to the nozzle models as Arina's (geometry based on Arina, 2004) and Wen's (geometry based on Wen et al, 2011), and we will use numbers to refer to the different central body designs, according to fig. 4 and fig. 5. While both nozzles and central body 3 are based on the geometries proposed in Arina (2004) and Wen et al (2011), the central bodies 1 and 2 are adapted from NACA series geometry profiles.

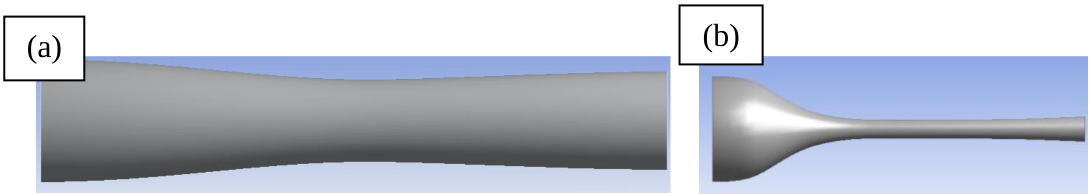

Figure 4. Nozzle models (a) Adapted from (Arina, 2004); (b) Adapted from (Wen, *et al.*, 2011)

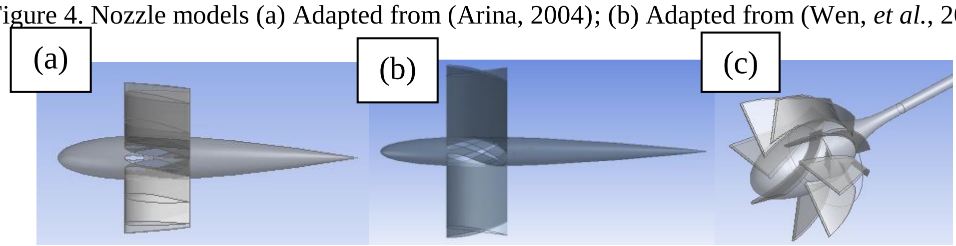

Figure 5. Central body models (a) Central body 1; (b) Central body 2; (c) Central body 3

3.1 Nozzles performance evaluation

At first, the two nozzle models were compared within a same base of boundary conditions (listed in table 3), and assuming the flow as inviscid, according to (Arina, 2004).

Table 3. Boundary conditions proposed by (Arina, 2004)

Parameter	Inlet	Outlet
Static pressure (kPa)	ND[(1)]	83.049
Total pressure (kPa)	104	ND[(1)]
Total temperature (K)	291.3	ND[(1)]

[(1)] not defined by user

The results of the invscid flow through the two nozzles are presented, respectively, in fig. 6 and 7. The stronger contraction of the Wen's nozzle allows higher cooling. Besides that, the shock wave position is more favorable for Wen's nozzle due to the longer length with low temperature that allows separation of gas components.

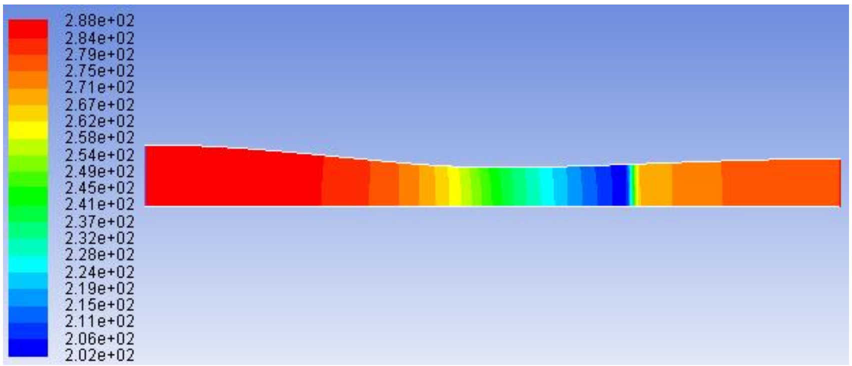

Figure 6. Contours of static temperature for Arina's Nozzle

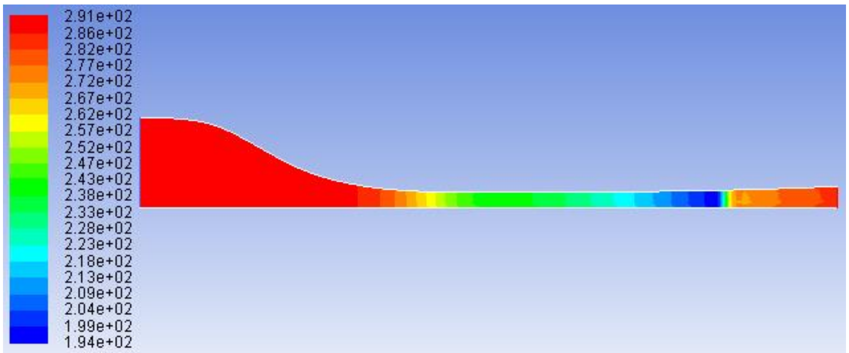

Figure 7. Contours of static temperature for Wen's Nozzle

From this point the central body is introduced, which is used to generate swirl into the three-dimensional nozzle. In this case the flow is assumed as viscous, and the k-ω SST turbulence model is applied to solve the RANS equations. Series of simulations were carried out to compare the three central body designs with a same base. Thus, in this study, a new set of boundary conditions were designated but keeping the static pressure ratio γ (as defined in Wen et al, 2014) fixed to 70%.

Table 4. Boundary conditions modified to pressure ratio 70%

Parameter	**Inlet**	**Outlet**
Static pressure (kPa)	ND[(1)]	70
Total pressure (kPa)	104	ND[(1)]
Total temperature (K)	291.3	ND[(1)]

(1) not defined by user

The analysis of figures 8 and 9 suggests that in terms of centrifugal force (which is a good performance index) Arina's nozzle with NACA cambered airfoils geometry performs best. However, according to (Twister BV, 2017) as shown in figure 2, centrifugal accelerations of the order of 500,000g are needed to separate the fluid components, but figure 9 shows that at the majority nozzle extent (downstream the nozzle throat), the centrifugal acceleration is still below 100,000g, specially at the region where the collector should be placed. This led to the necessity of studying methods for optimization.

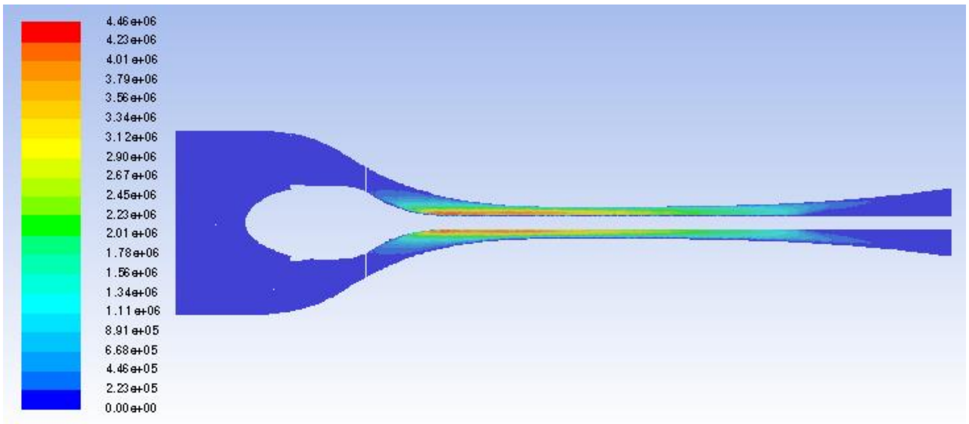

Figure 8. Contours of centrifugal acceleration at a longitudinal cross section for Wen’s nozzle design

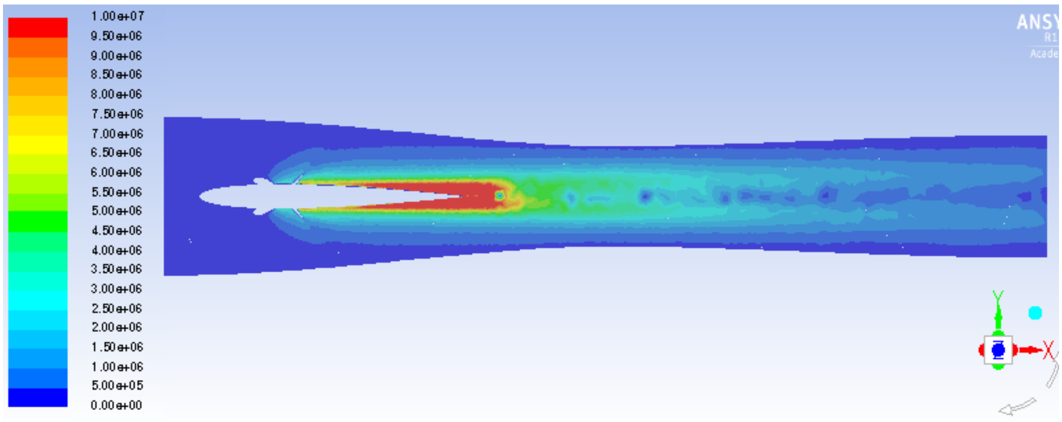

Figure 9. Contours of centrifugal acceleration at a longitunal cross section for Arina’s nozzle design

Although the implementation of Wen’s design model was successful in terms of reaching close levels of performance regarding to (Wen, *et al.* 2011), due to its vanes complexity and the lack of information about modelling parameters, the optimization study will be restricted to Arina's nozzle design.

3.2 Genetic algorithm implementation

The primary step to implement the optimization algorithm is to identify the relevant degrees of freedom of the problem. Firstly they were divided between similar and disparate, which are disclosed in table 5. The first column refers to parameters that comply with similarity conditions, so their influence will be neglected in the optimization, as they can be predicted with non dimension analysis. The second column, instead, refers to parameters that break the geometry similarity, thus they are the degrees of freedom for optimization. In order to maintain the base for comparison, all simulations within this section applies table 4 boundary conditions.

Table 5. Similar and disparate degrees of freedom

Similar	**Disparate**
Pressure ratio	Central body scale
Total enthalpy	Helix number
Inlet pressure	Angle of Attack
Global scale	Central body position

The quality of a good optimization relies not only on the method employed, but mostly in the precise definition of the objectives. Therefore, since the goal of the project is not just reach higher swirl intensities, but also maintain high cooling power, a multi-objective scheme was employed, using the Pareto border approach, to maximize both the tangential velocity area average on collector’s cross section and also the Mach number, which is directly related to the cooling power.

The genetic algorithm effectiveness also relies on the definition of a set of parameters and their range, which will determine the set of genes, and consequently the extent of the searching locus. Preliminarly, a serie of simulations were carried out to find which conditions the flow through the vanes would stall, due to the fact that at these situations the flow losses would be more significant in face of the high level of flow fluctuation and turbulence. However, it is expected that just before stalling, the flow should be at its maximum capability of both cooling and swirling. Thus, by means of the simulations carried out with a fixed pressure ratio (gamma), taking into account the nozzle efficiency in terms of cooling and swirling capabilites, a set of parameters were selected to be considered for the optimization study as shown in table 6.

Table 6. Selected parameters used for the optimization study.

Parameter	**Range**	**Description**
Helix number	(12;14;16;18)	Number of vanes of the central body
Attack angle	(24º;26º;28º;30º)	How many degrees the airfoil is rotated in relation to the central body
Scale	(25%;30%;35%;40%)	Size reduction of the vanes in relation to the central body
Position	(12;14;16;18)	Placement (in millimeters) of the vanes with respect to the central body

For each set of parameters a proper chromossome is designated, for instance the chromosome [1,2,0,3] corresponds to the design with 14 airfoils, attack angle of 28º, scaled by 25% and positioned at 18mm from the origin.

As the genetic algorithm method is not deterministic, every run (pareto optimal approach, see section 2.2) gives rise to a new pareto border with potential slight differencies. Thus in order to attest the convergence, the entire routine was run five times (which required the calculation of 150 out of the 256 individuals of the searching locus), so that the individuals present in all the Pareto border generated are shown in table 7. Finally, the intermediate individual ([0,3,0,1]) was chosen to be the best, as it combines good performance for both objectives, as shown in figures 10 and 11.

Table 7. Pareto border results

Chromosome	**Tangential velocity average [m/s] (Objective 1)**	**Mach Number (Objective 2)**
[0,1,0,3]	67.25	1.51
[0,1,0,2]	67.62	1.50
[0,2,0,2]	71.50	1.46
[0,3,0,1]	74.20	1.45
[2,3,1,3]	78.95	1.43
[1,3,1,1]	81.50	1.36
[1,3,1,2]	83.34	1.35

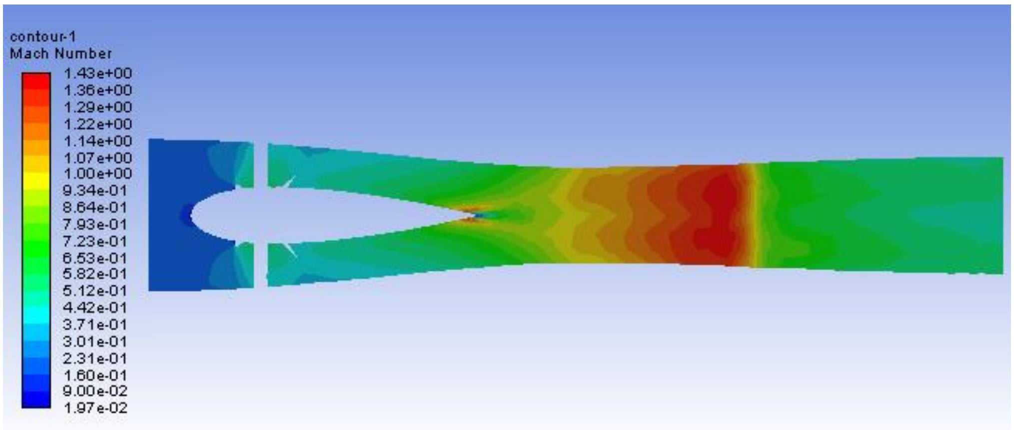

Figure 10. Countours of Mach number for best individual.

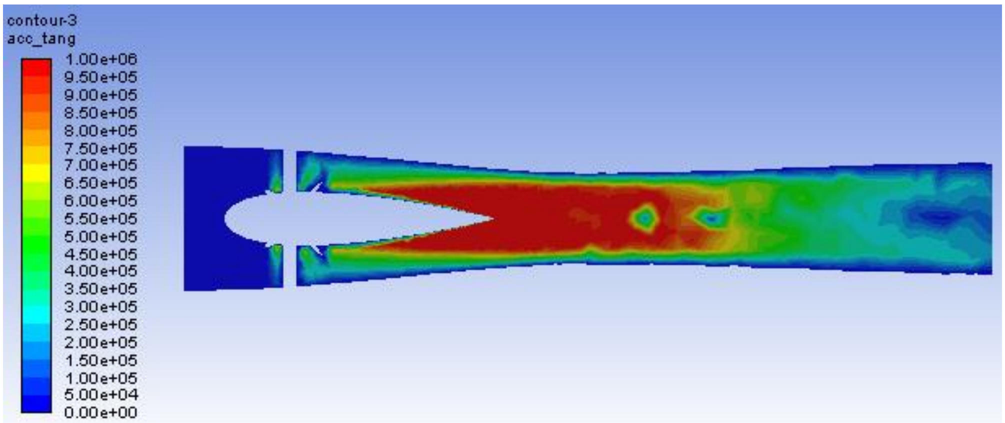

Figure 11. Contours of centrifugal acceleration for best individual

Overall, the algorithm has its strength in the capability of dealing with high nonlinear problems, but also shows some weaknesses such as a absence of a realiable stop criteria, which affects its efficiency. This is even more evident on implicit problems, whose fitness evaluation process consumes much time. Furthermore, some factors such as the inexistence of a unique definition of the collector's position within the separation zone (which may vary with the shock wave position), as well as the variations of the mesh quality for each run (as the geometry changed), could have affected the precision of the method on finding the best set of individuals

4. CONCLUSIONS

This project achieved its main objectives by first exploring the flow dynamics inside supersonic separators, modelling not just the main geometry types that compose the state of art, but also introducing the swirl generators. We present information concerning the swirling and cooling properties of the different designs, identifying the need for better performance, and implemented an optimization routine based on Genetic Algorithm method.

5. ACKNOWLEDGEMENTS

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