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TURBOMACHINERY DESIGN: CHECKING ARTIFICIAL NEURAL NETWORKS SUITABILITY FOR DESIGN AUTOMATION

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ABSTRACT

This paper explores the suitability of Artificial Neural Networks (ANNs) as an enabler of Design Automation in the turbomachinery industry. Specifically, the paper provides 1) a preliminary estimation of the effectiveness of ANNs to define values for design variables of reciprocating compressors (RC) and 2) a comparison of ANNs performance with traditional and more computationally demanding methods like CFD. A tailored ANN trained on a dataset composed by 350+ Baker Hughes' RC automatically assigns values to 8 geometrical variables belonging to multiple parts of the RC in order to satisfy two target conditions linked to their thermodynamic performance. The results highlight that the ANN-assigned parameters return an optimal solution for RC also when the target values do not belong to the training dataset. Their predictive capacity for RC thermodynamic performance, with respect to CFD, are comparable (i.e. less than 2% in terms of calculated absorbed power) and the approach enables a significant gain in terms of computational time (i.e. 2 minutes vs 10 hours). Future perspectives of this work may involve the integration of this tool in an advanced DA method to lead Design Engineers (DEs) during the whole design process.

Keywords: Artificial intelligence, Computational design methods, Embodiment design, Turbomachinery, Optimisation

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1 CONTEXT AND RELEVANT BACKGROUND

The turbomachinery industry is currently undergoing rapid innovation in design concepts due to the emergence of new energy transition markets. As a result, energy companies are required to quickly redesign their products to meet the evolving needs of their customers. To achieve this, the product engineering development of turbomachinery components requires a multi-disciplinary design approach, including parametric CAD modelling, Finite Element Structural Analyses (FEA), Computational Fluid-Dynamics Analyses (CFD), and thermodynamics. Many turbomachinery companies adopt an Engineering-To-Order (ETO) production approach, which means that key design-related activities must be completed within a short lead time after receiving a customer order. These activities involve iterations of calculations and design analyses that sometimes involve data and constraints that are not fully known at the outset.

The traditional trial-and-error design method used in most activities of the product development process depends on the experience of Design Engineers (DEs). This approach cannot lead to globally optimized designs and typically results in very long design cycles (Li and Zheng, 2017). For ETO engineering companies, it is essential to automate its internal processes, particularly during the engineering design phase, which is at the core of their business. In order to reduce errors and delays, as the market demands, design methods and tools offer an opportunity to shorten the design phase making it more efficient (e.g. by avoiding time consuming iterations).

Design Automation (DA) solutions are widely used in the industry to increase product competitiveness in the market and improve overall company productivity. The adoption of Knowledge-Based Engineering (KBE) in the early design stage can lead to standardization, error reduction, and a reduction in lead time (Ascheri et al., 2017). KBE can also increase the efficiency of product manufacturing and reduce time-consuming and repetitive tasks (Lindholm and Johansen, 2018). However, a limitation of DA applications is the need to choose from automatically generated alternative solutions (Entner et al., 2019). Moreover, the design space size formulation is only valid for a sub-space within which only some morphological transformations are allowed. This is a substantial limitation, as DA models cannot exceed the constraints within which they have been developed (Amadori et al., 2012).

To overcome this limit, several methods attempt to find optimum designs using techniques that avoid following a specific defined solution. Furthermore, in the engineering design process of ETO-structured companies, there can be the necessity to avoid exploiting gradient or quasi-gradient information to respond as quickly as possible to changes in inputs or constraints. Among the techniques meeting these needs, there are processes which either exploit randomised variations in the design variables or avoid the direct modification of design variables altogether by using learning networks. Among the first group, there are the Guided Random Search Techniques (GRST), i.e. Genetic Algorithm (GA), and similarly, for the second group, there are the learning network-based methods, i.e. Artificial Neural Networks (ANNs). GAs are a family of computational methods inspired by the Darwinian/Russel Wallace theory of evolution applied to solve general optimisation problems (Sobieszczanski-Sobieski et al., 2015). ANNs are a very simplified model of the human brain, depicted as having billions of neurons, each connected to several thousand other neurons (Bishop, 1994). The computational cost of GAs and ANNs depends on the problem and the specific implementation. GAs may be more expensive when dealing with large search spaces or discrete optimisation problems, while ANNs may be more efficient for function approximation or regression tasks (Che, 2011).

The essential properties of biological neural networks from the viewpoint of information processing will allow us to design abstract models of artificial neural networks, which can then be simulated and analysed after their training on more or less large quantities of data available (Rojas, 1996). In recent years, ANNs have been applied to a lot of industrial problems, from functional prediction and system modelling (where physical processes are not well understood or are highly complex) to pattern recognition engines and robust classifiers, with the ability to generalise while making decisions about different kind of input data (Meireles et al., 2003).

In the literature, the first applications of ANNs in the turbomachinery industry concern the simulations of design and off-design conditions of gas turbines operability (Lazzaretto and Toffolo, 2001), the prediction of axial compressors performance map (Yu et al., 2007), and the centrifugal compressors performance (Jiang et al., 2019). This approach, however, gives an estimation of the performance of the

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single components without taking into account the effects of the variations of internal design parameters on performance. A comparison between ANNs and other metamodels able to predict the performance of axial compressors has been carried out by Ghorbanian and Gholamrezaei (2009). In the last years, ANNs have also been used for the optimisation of components layout (Du et al., 2022) and, in general, for design optimisation of turbomachinery components as a surrogate model to avoid huge computational efforts typical of more robust optimisation methods (i.e. GA) when a big number of data is available (Woldermariam and Hirpa, 2019). Applications have been carried out on centrifugal impellers (Ji et al., 2021), radial turbines (Luczynski et al., 2021) and fan blades (Lopez et al., 2021).
ANNs applications in advanced DA models might trigger advantages as they enable the quick processing of large amounts of data and the engineering practice showed they could be effective when it is difficult to identify, a-priori, a suitable design optimisation model. The main disadvantage arises when the network must respond to inputs substantially different from those used for its training or in case the results are expected in regions of the design space where the inputs are significantly different from those used in the training phase, as described by Bishop (1994).
In fact, in order to contribute to filling the above-mentioned research gaps in the ETO turbomachinery industry, the aim of this work, developed in partnership with Baker Hughes (BH) engineering department, is to provide an estimation of the multi-objective predictive capacity of the ANN method for BH Reciprocating Compressor (RC) cylinders and to compare it in terms of performance calculation and computational time with respect to more computationally demanding methods like CFD. The choice to explore ANNs predictive capacity is due to the nature of the design problem, as the cylinder's topology directly affects its performance, and because of the availability of a dataset that contains data about RCs' topology and the related thermodynamic performance, as estimated through extensive CFD analyses conducted in the past years. This dataset represents the design space of the existing cylinder families. Indeed, due to the large amount of miscellaneous data already present in the BH database, it may be advantageous to use ANNs to construct a surrogate model of the problem instead of more computationally demanding numerical methods. Hence, the paper intends to answer the following question: how do ANNs perform in terms of predictive capability and computational time with respect to traditional more time-consuming simulation methods, when dealing with non-routine design covered by pre-defined DA models, which represents RC cylinders?
Section 2 frames the method for non-routine RC cylinders design as a process that integrates the application of ANNs in order to overcome the main challenges of ETO-structured business. This section includes details about the RC data provided in the dataset, a description of the ANN specifically developed for such study and its integration in the workflow via an orchestrator which enables DEs to target goal parameters of the desired configuration with the related Key Performance Indicators (KPIs). Section 3 describes the application of the method in a case study related to a non-routine design of a new BH RC cylinder, by highlighting the results according to the KPIs. The last section summarises the results, with an overview of the scientific contribution of this work, its limitations and the future research perspectives.

2 METHOD

2.1 RC cylinders design in the ETO process

The current design development process of RC cylinders is primarily human-driven and iterative, with design changes made as needed to meet technical and organizational requirements. This work proposes a tool to optimize the design of RC cylinders by targeting customer needs for optimal solutions and fast turnaround times. The ETO RC cylinder design process is driven by engineering requirements and involves modifying features and geometrical characteristics that affect the mechanical and thermodynamic performance of the machine. Given the importance of these factors, this work aims to test the validity of ANNs as an alternative to computationally expensive CFD analysis for RC cylinder design. The goal is to assess the reliability and the time-saving potential of ANNs for this application. Figure 1 shows the section of an API 618 BH RC. The right end of the picture highlights the cylinder, which is the group of this reciprocating compressor this work focuses on.

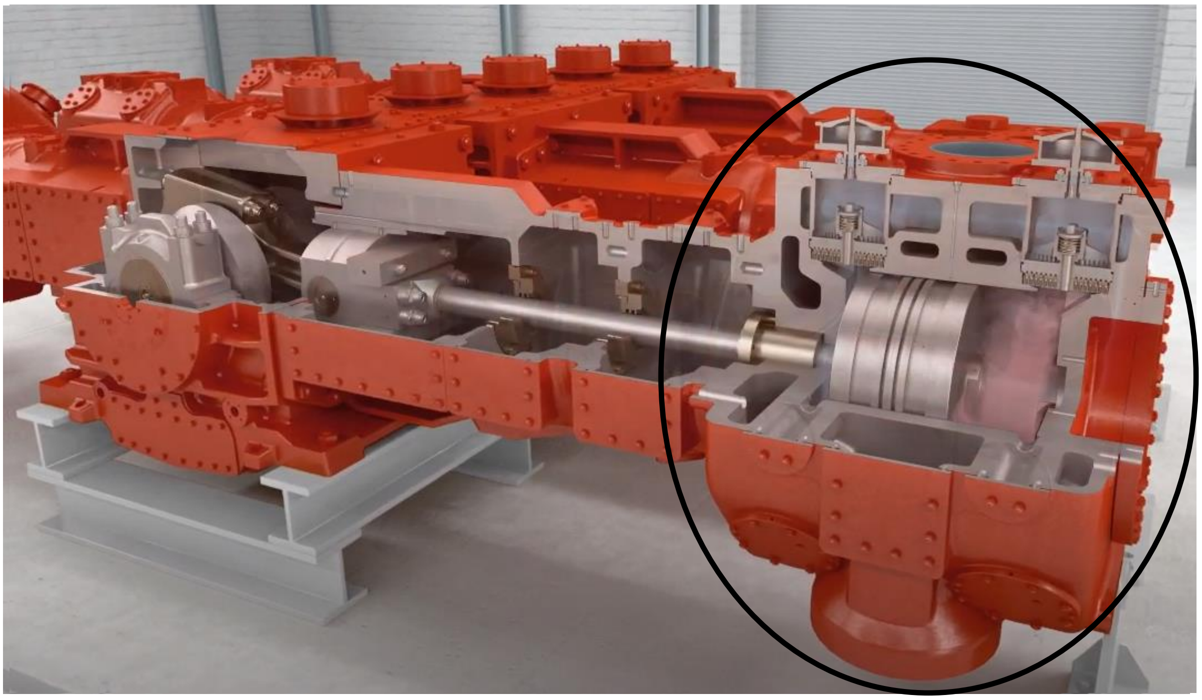

Figure 1. Section of an API 618 BH reciprocating compressor.

One of the most critical issues in the design of reciprocating compressors is the pressure loss generated as the gas flows through the gas ducts and, in particular, in the section of the valve pocket, including valves and gas ducts between them and the compression chamber. The limitation of such waste of energy is crucial in the design of the valve pocket. Therefore, its evaluation becomes critical for the analysis of the cylinder performance mainly for two reasons:

- The pressure drop observed in the valve pocket is an index of the valve's effectiveness, as it affects the amount of work required to compress the gas.
- The relationship between the pressure drop and the mass flow rate must be known during the entire cylinder design process, since it is the base of the mathematical model for calculating the p-V cycle characteristic of the compressor.

The other key factor that affects the volumetric efficiency of the machine (and, therefore, its performance) is the presence of clearance volumes (or dead volumes) inside the cylinder. When the piston reaches the top dead centre at the end of the discharge phase, part of the volume presents not compressed gas. The effect of the clearance volumes on the reduction of the suction capacity is greater the higher the clearance volume itself and the compression ratio.

2.2 Dataset development and analysis

The cornerstone that makes it possible to check the performance of ANNs for non-routine RC design is the large database developed by BH. It includes the company's entire fleet of RC cylinders, composed of more than 365 different cylinders. Each of the RC therein collected is also provided with the results of CFD simulations and analyses. The results of CFD returned the global losses of each machine, this is summarised as the global flow coefficient K_s and as the clearance volume value ε. The flow coefficient $K_s = \frac{\dot{m}_{real}}{\dot{m}_{id}}$ is the ratio between the real and the ideal gas flow rate through the RC valves. This coefficient represents the factor necessary to reduce an ideal mass flow rate of an ideal gas through a given valve to obtain the real mass flow rate through the same valve once the pressure drop has been set. The clearance volume $\varepsilon = \frac{V_{TDC}}{V_C}$ [%] is the ratio between the volume remaining between the piston, the cylinder head and the valves of a RC cylinder when the piston reaches the top dead centre V_{TDC} [mm^3] and the cylinder capacity V_C [mm^3]. These are the two parameters which can be monitored by DEs to assess the performance of the RC cylinder. They are the two main inputs for the mathematical calculation of the absorbed power declared to the customer. Indeed, this is function both of K_s and ε.

$$\mathrm{P_{ABS}} = f(K_s, \varepsilon) \tag{1}$$

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The simulations needed to obtain these values required many hours of computational time (i.e., ~10 hours for a single cylinder). In the past, in fact, most of the studies were focused only on the analysis of the pressure losses of the valves, while today the losses of all the other components of the machine have also assumed vital importance, as the gas ducts layouts has undergone changes over time. The use of CFD simulation has shown great potential for studying the entire reciprocating compressor but is still limited by high computational costs. The timing of such analyses is primarily incompatible with BH ETO process schedule, as often it is not possible to dedicate resources and computational time of such order of magnitude for this purpose. For this reason, there is a need of scouting innovative methods to find design solutions of RC cylinders able to respond as quickly as possible to customer requests.
The database used for this work, available on BH systems include, for every cylinder:

- Cylinder code, which uniquely identifies the single cylinder.
- Cylinder bore.
- Cylinder valves number and size.
- 6 geometric parameters which describe the gas flow path topology. Among these, there are distances, angles, dimensions of components which affect the performance of the cylinder in terms of K_s and ε.
- K_s for both suction and discharge phase, both at the head and crank-end of the cylinder.
- ε both for the head and crank-end of the cylinder and the medium value.

The BH database has been rearranged with the following simplifications for the purpose of this analysis:

- K_s takes the value it gets at the head-end side of the suction phase.
- ε is averaged considering both the head and the crank-end side of the cylinder.

That is, for simplicity, only the suction phase of the head-end side of the cylinder has been analysed. The database has been rearranged in this way, for a total of 8 independent parameters, two dependent variables (K_s and ε) for each of the 365 different cylinders embedded in the original database
Some variables, such as the number and size of valves, are discrete and have standard values. However, other variables are represented as discrete geometrical values that could theoretically be continuously altered by an artificial neural network (ANN). Based on the analysis of this heterogeneous database, the physics of the problem, and the literature reviewed in Section 1, a metamodel will be developed to represent the independent variables that affect the two dependent variables. This metamodel (i.e. the ANN) will be presented in the following section.

2.3 ANN training and ANN performance estimation

The database has been prepared and imported in MATLAB, which has been chosen together with BH IT department as the most suitable tool for this exploratory analysis. Training multiple neural networks and averaging their results can improve the performance and generalization of the model compared to training a single neural network. This is known as model ensembling, and it has been shown to be an effective technique in machine learning (Yu et al., 2008). Training a single neural network on a large dataset can lead to overfitting, where the model becomes too complex and starts to memorise the training data instead of learning the underlying patterns. However, averaging the results of multiple neural networks can help reduce overfitting, as each network will learn slightly different representations of the data and averaging them will produce a more robust and generalized model. Then, averaging the results of multiple neural networks can improve the accuracy of the model, as the individual networks may make different errors on different parts of the dataset. By averaging their predictions, the errors can be dampened, leading to a more accurate overall prediction. Finally, it is important to know how uncertain the model is about its predictions. Averaging the results of multiple neural networks can provide a more reliable estimate of uncertainty, as the ensemble is more likely to capture the full range of possible outcomes. Overall, training multiple neural networks and averaging their results can help improve the performance and robustness of the model, especially when dealing with large and complex datasets.
With this purpose, a sensitivity analysis on the number of ANNs and size of the hidden layer has been carried out. Time consumption for training and execution of one calculation together with results comparison have been evaluated for 10, 20, 30, 50 and 100 ANNs with hidden layer size 10, 20 and 30. Results do not considerably vary with more than 30 ANNs with size 20, while the time consumption continuously increases. For this reason, 30 feedforward ANNs with one hidden layer of size 20 (Figure 2) have been created and trained to avoid biases and minimise errors. The output values are the mean values computed by 30 ANNs.

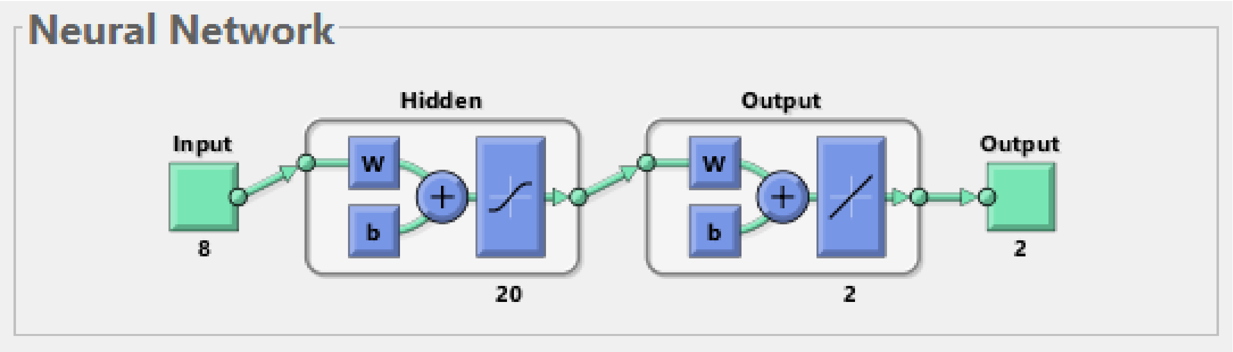

Figure 2. Representative ANN scheme on MATLAB.

As Ks and ε values affect the performance of the RC machine declared to the final customer, it is necessary to assess the impact of the error in terms of absorbed power. The quality of the ANNs has been checked by comparing the outputs computed with the ANNs and the same sample of the dataset. The Mean Absolute Percentage Error (MAPE) represents a measure of the prediction accuracy of a method. It has been calculated for both the variables K_s and ε.

$$\mathrm{MAPE}_{\mathrm{K_s}} = \left(\frac{1}{n}\sum_{i=1}^{n}\left|\frac{K_{s_{DTR}}-K_{s_{NN}}}{K_{s_{DTR}}}\right|\right) = 0.1\ \% \tag{2}$$

$$\mathrm{MAPE}_{\varepsilon} = \left(\frac{1}{n}\sum_{i=1}^{n}\left|\frac{\varepsilon_{DTR}-\varepsilon_{NN}}{\varepsilon_{DTR}}\right|\right) = 1.43\ \% \tag{3}$$

Where $K_{s_{DTR}}$ is the value of K_s present in the database, $K_{s_{NN}}$ is the value of K_s calculated with the ANNs, ε_{DTR} is the value of ε present in the database, ε_{NN} is the value of ε calculated with the ANNs and n is the number of samples present in the database.
The observed 0.1% MAPE for K_s and 1.43% for ε lead to a 0.1% error on the declared absorbed power, which has been considered acceptable as the customer accepts a large enough tolerance on that value, with respect to the one resulting with the above-mentioned MAPEs.

2.4 ANN as a DA enabler

The trained and validated ANNs have been embedded into a tool that delivers the optimal solution once the computational goals have been set. Isight (Van der Velden et al., 2010) is an orchestrator used to combine multiple models and multi-disciplinary applications into a simulation process flow, automate execution across distributed computing resources, explore the resulting design space and identify optimal design parameters responding to the required constraints.

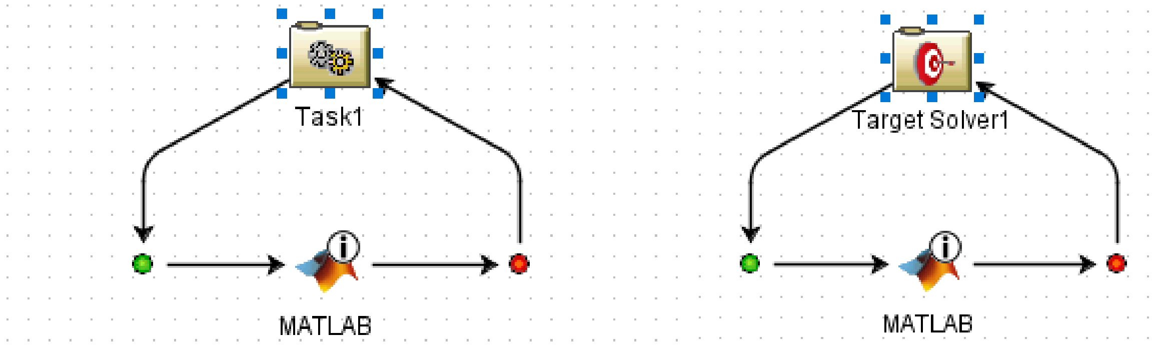

Figure 3. Base loop of MATLAB ANNs integrated into Isight (left). ANNs integrated into the target solver component (right).

This basic loop "Task1", shown in Figure 3 on the left, allows to orchestrate the above-described ANNs to automatise the cylinder layout update according to different customer requirements and to read the results in a user-friendly manner. It orchestrates the input values manually inserted by DEs by running the Matlab routine, which embeds the ANNs shown before. In the case of the cylinder model that has been built in this study, a direct evaluation of the performance of a certain configuration can be carried out in this way. In the components tab of Task1 the baseline value of the parameters of the desired

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configuration can be set. The outputs are the values of K_s and ε obtained through the metamodel (i.e. ANNs) of the related cylinder layout. This process can be furtherly improved using the Target Solver component which is present in Isight (Figure 3, right). The Target Solver component in Isight changes the baseline value of variables within a specified range until the target values of the model are reached (within a specified tolerance) or until it exceeds the specified number of evaluations.

This component runs the ANNs embedded in the Matlab routine already presented with this goal. The Target Solver is particularly useful for solving a system of equations made up of target parameters, like in the case of this analysis. This component in Isight is used to specify the target values of a set of output parameters and select the variables that will be modified to reach these values. In the Targets table the goal values of K_s and ε are set.

In the Variables table the different variables of the design space are edited. There is the possibility to choose which variables will be modified by the tool and the range within which they can vary. The output of this run is the set of parameters of the optimised RC cylinder assembly, which has to be exported manually in the 3D CAD software by DEs to deliver the optimal configuration able to respond to the customer needs in terms of K_s and ε.

2.5 KPIs of the method

As the competitiveness of BH RCs in the market is defined by their own performance and cost, it is important to assess the output of the method presented in this research within a certain interval of tolerance (i.e. BH declares the calculated absorbed power to the customer with a certain tolerance), by minimising the computational time. For this reason, in order to answer to the research question formulated in the introduction, the KPIs of the process according to which the quality of the tool described above will be evaluated are:

- Functional performance, defined as the "quality" of the output in terms of error with respect to the benchmark (i.e. CFD analysis), measured on the values of Ks and ε.
- Computational time to deliver the optimised solution to the customer, with respect to CFD analysis.

3 COMPUTATIONAL APPLICATION

3.1 Cylinder description

In order to answer the research question, a case study related to a BH RC cylinder has been carried out. It is representative of a real ETO activity in Baker Hughes. In particular, it reflects a real case study: a new customer needs a RC to face the energy transition. With reference to the research question presented in the introduction, indeed, the purpose is to prove that ANNs can be a valid alternative to more expensive optimisation methods like CFD, which has been considered the benchmark of the analysis. The cylinder (Figure 4) is part of a BH new product development program that might answer the new customer demands, but which is lacking an appropriate configuration to meet its requirements. Such cylinder can be considered a scaled up version of one of the existing RCs that trained the ANNs. In other words, the overall geometrical characteristics of this cylinder are similar to the ones of the cylinders belonging to the training dataset, especially in terms of shape of the gas ducts. The size and the number of the valves are standard, but the combination of their values with the internal bore and the dimensions of other components place this cylinder outside the boundaries of the design space which the dataset is based on. This makes this analysis suitable to estimate the capability of the approach to reach thermodynamic performance that are similar to the one of the same family, which results in target values of K_s and ε.

3.2 Computational path

The computational path is herein summarised. The DE sets the goal parameters of K_s and ε of this case study in the Targets tab of the Target Solver Editor of Isight, which runs ANNs with the methodology explained in 2.3. The other eight parameters have been modified by the tool to reach the final configuration able to respond to the requirements. The final parameters are manually exported by the DE in the 3D CAD software to obtain the optimal configuration of the cylinder. With this configuration, a complete CFD analysis has been carried out as a reference value to verify the KPIs of the study. The results are:

- The comparison of the two values for K_s, i.e. the one estimated by the ANN ($K_{s_{ANN}}$) and the one obtained by means of the simulation using a CFD model($K_{s_{CFD}}$), shows that the relative error is 0.3%. Furthermore, for what concerns ε, the relative error between the metamodel (ε_{ANN}) and the CFD simulations (ε_{CFD}) is 8.7%. As both these values affect the absorbed power, the estimation of the error for this quantity is 1.7% (which is within the interval of tolerance declared by BH to the customer). The results obtained with the ANNs are the mean values of the surrogate model developed through the methodology described in 2.3.
- The computational time to deliver the optimal configuration with ANNs is 2 minutes vs around 10 hours needed to run the CFD model.

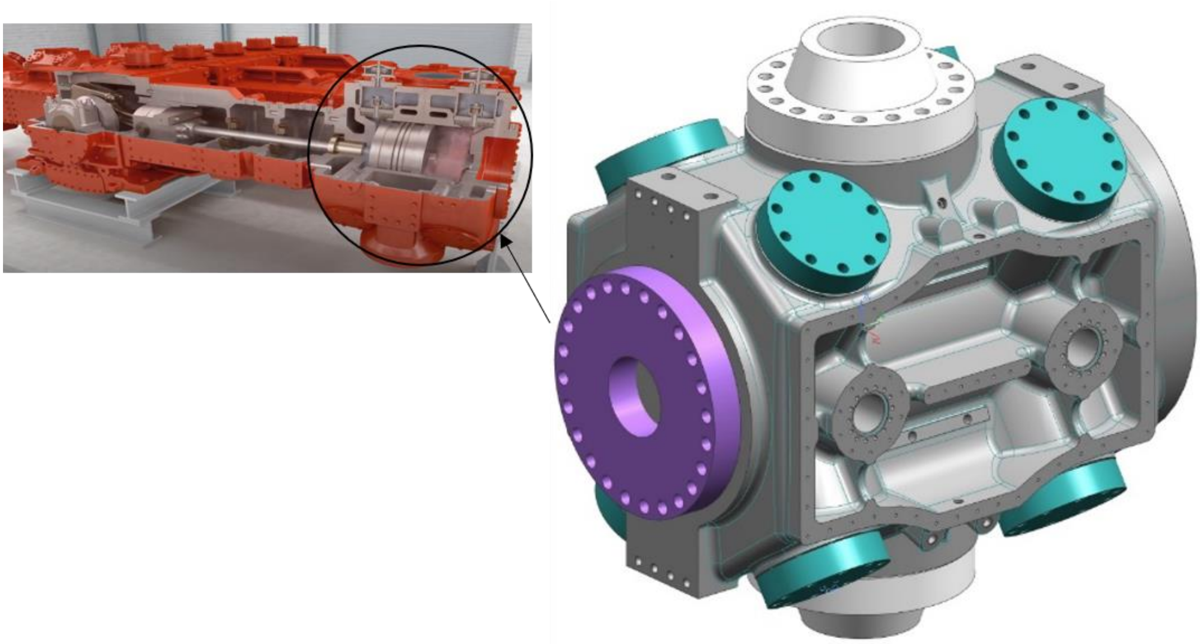

Figure 4. New BH RC cylinder assembly.

4 CONCLUSIONS AND FUTURE PERSPECTIVES

This paper presents an application of ANNs for a DA solution related to systems of turbomachinery components capable of supporting DEs in delivering a nearly-optimal design solution trough a computational time reduced by two orders of magnitude with respect to CFD analyses. In particular, the final configuration of the target system (i.e. RC cylinder assembly) is developed seeking goal values of a multi-objective function, related to the performance of the machine itself. An application of this metamodel to a case study representative of a new BH product is shown, with the purpose of validating the hypothesis that ANNs are sufficiently capable to predict and properly assess the performance of the cylinder (and so of the whole machine), with respect to more time-consuming CFD models.

The results are summarised herein. Through the analysis of these results shown in 3.2, it emerges that ANNs are a promising tool for supporting BH DEs where non-routine design is required in a short time, as for their ETO-structured business process. Indeed, ANNs allow reaching the final configuration within a few minutes without the necessity of running complete CFD models. These results also show that this metamodel is capable of delivering the optimal solution outside the boundaries of the training set with sufficient predictive quality. This aspect is of particularly great importance when dealing with the development of new products in a short period of time, as, for instance, it is required for energy companies facing the energy transition. In order to better highlight the limitations of design applications of ANNs in terms of shape and dimensions, it seems to be useful to extend the approach described in this research to different families of RC cylinders. For example, it may be possible to understand how to modify the ANN metamodel developed for the purpose of this work (i.e. re-training with a new dataset).

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As per the work presented, the main limitations of the ANNs tool presented in this paper are summarised in the following three list items:

- The training of ANNs is carried out using values that approximates the real behaviour of the machine via averaging or by means of cut-off criteria (e.g. average values of clearance volumes may lead to significant errors in the prediction of ε).
- There is a lack of self-learning of the ANNs after each computational path.
- Training has been done on a finite number of parameters which does not allow design exploration outside the design space of the same type of geometry ruled by a model.

A possible improvement of the presented ANNs tool's predictive capacity may involve the development of a metamodel representing a complete RC cylinder without approximations needed on clearance volume values (which appear to be the main contributors to errors in absorbed power calculation). Furthermore, the implementation of self-learning metamodels may lead to an increased predictive capacity of machine learning techniques with respect to the one presented in this work.

Finally, another possibility may be the development of an advanced integrated DA method able to lead DEs in meeting design requirements and customer needs with a robust approach, implementing DA master models in a product configurator to be optimised by the ANNs orchestrated by Isight as per the presented work, to obtain the required final configuration of the cylinder, which can be then included in the final overall thermodynamic and mechanical calculation of the whole compressor.

In any case, machine learning can help BH improve efficiency and reduce costs in its engineering activities. The company has already started by identifying the areas where machine learning can have the most significant impact and investing in the necessary data infrastructure and talent to implement these solutions.

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