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Computational Models for the Analysis of positive displacement machines: Real Gas and Dynamic Mesh

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Abstract

In recent years, computational fluid dynamics (CFD) has been applied for the design and analysis of positive displacement machines (both compressors and expanders) with numerous challenges due to the dynamics of the compression (or expansion) process and deforming working chambers. The relative motion and in turn, the variation of the gaps during machine operation implies several obstacles for the implementation of reliable CFD models. The majority of the studies reported in literature focused on scroll, twin screw and reciprocating machines. The limitation of the developed methodologies to be applied directly to positive displacement machines with more complex meshing such as that of single-screw has been highlighted in literature.

In this paper, a single screw expander is studied by means of (i) a moving mesh technique (dynamic mesh in the Key Frame Remeshing approach) and (ii) a real gas model of a R134a (Peng-Robinson model) implemented in OpenFOAM[®]. On the top of that, all the possible techniques that come with the software are investigated in their application to single screw. An useful review of the state of the art CFD with open-source software (OpenFOAM-v1606+ and foam-extend4.0) is therefore carried out. The reliability of CFD model represents indeed the first step on which the design process and further optimization will be based.

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1. Introduction

Today the demand of efficiency in the recovery of thermal power and conversion in mechanical power is pressing. Pushed by the high costs of the fuel and above all by the increasing amount of CO₂ in the air, the request of a better and more responsible use of the waste thermal energy is in the spotlight. In this framework, that is the pursuit of

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more efficient ways of utilizing existing technologies, ORC systems are one of the best candidates to achieve the goal. During recent years, organic Rankine cycle systems have gained maturity, becoming a widely accepted technology to convert low grade heat into electricity [1].

Perhaps the most interesting component of the cycle is the expander. In the available applications both dynamic and volumetric machinery are employed. The problem with turbines is that both the unsteadiness of the conditions at which the waste energy is available (in case the machine is applied to Internal Combustion Engine cogeneration, [2]) and the low enthalpy jump can cause dramatic efficiency losses. Positive displacement machines are therefore widely used in ORC systems as expanders replacing turbogenerators for micro-ORC applications [3]. Within this framework, the performance of the ORC system should be optimized by choosing the right expander geometry and operating conditions [4].

This work mainly focuses on micro ORC systems, when the power output of the cycle is lower than 100 kW. If this is the case, among all the available machines, alternative and screw expanders are the most used ones. For what concerns the latter, they can be divided into two categories: single-screw expanders (SSE) and twin-screw expanders. Recently, researchers have started looking into single-screw expanders as an alternative to twin-screw expanders. Among the other reasons, their balanced loading on the main rotor and wide range of operation [5] make their application very attractive. Promising results are reported by Wang *et al.* [6] and Lu *et al.* [7]. In the first case an adiabatic efficiency of 59 % was achieved with a maximum power output of 5 kW. The authors report that efficiency could be increased by improving the lubrication and the low value of efficiency obtained is also due to the use of dry air. In the latter case, with a 175 mm diameter rotor, the SSE reached an adiabatic efficiency above 65 % using a compressed air refrigeration system.

The Computational Fluid Dynamics (CFD) analysis [8–11] is a useful tool for the prediction of flow behaviour and performance: the geometry complexity and the compatibility of the instrumentation make the experimental campaign very challenging. Sometimes the numerical approach is the only way to investigate the potential behaviour of the expander with new fluids without major changes to the plant to be carried out. Nonetheless, such simulations are quite complicate. The complexity of the simulation has brought about the application of several numerical strategies to solve the behaviour of volumetric machinery. Among the others machines, the SSE is particularly difficult to be simulated. Particularly tough is the meshing phase of the simulation: the definition of a structured grid compatible with the rotors displacement is not straightforward. Such a mesh could bear the high deformation and the stretch imposed by the motion without seeing a drop in the cell quality. Indeed few attempts in the literature have been done in simulating such machinery, basically taking advantage of overset grids [9].

In this article many approaches for the analysis of single screw expanders through CFD are illustrated. All the possible approaches that come with the open-source software OpenFOAM-v1606+ and the extended version foam-extend 4.0 have been tested on the case study. The peculiarities of all the studied techniques are reported and the main features of each approach are highlighted.

The numerical approaches investigated are:

- Immersed boundary
- Mesquite - Adaptive Remeshing
- Key-Frame-Remeshing

The approach chosen for the simulation must cope with the model for the elaborated fluid. Seldom the gases that are employed in this kind of machinery follows the ideal gas behaviour. As reported in [2], the ideal gas model still holds only if the working conditions are far from the critical point. If this is true the collisions between gas molecules can be considered perfectly elastic. Closer to the critical point the intermolecular forces cannot be neglected and thus the ideal gas approximation must be dropped. Considering the gas to have the ideal behaviour in the proximity of the critical point can lead to deviations up to the 12 % in the performance prediction, as reported by [2].

The appropriate model of real gas should rather be chosen, according to experimental data available or comparison with numerical code that implement the Helmholtz equation [12]. In this work the Peng-Robinson model [13] is used.

This work is intended to be an overview of the available methods to numerically simulate single screw expanders and in general positive displacement machines with open source software. In this paper the possibility of using

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