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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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Keywords: Single Screw Expander; Meshing Techniques; Real Gas Expansion; OpenFOAM;

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 CO_2 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 brough 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

OpenFOAM-v1606+ and foam-extend4.0 with this purpose is illustrated. Particularly, the application to a small scale single screw expander is investigated.

2. Methodology

In the following the main features related to the numerical simulation of the SSE will be listed. Extra care will be given to the problems which typically represent the biggest challenges in this field, namely the dynamic mesh motion solver and the real gas modelling.

2.1. Geometry and Meshing tool

The machinery investigated in this work is representative of a small size single screw expander elaborating R134a. The geometry of the rotors is reported in fig. 1. A six-grooves screw (rotating at 3000 rpm) engages with two eleven counter-rotating-teeth star wheels providing an overall pressure jump of 6 bar. The inlet conditions are p=1.2 MPa and T=400 K. Such conditions locate the working point not far from the critical point (p_c=4.07 MPa and T_c=374.3 K) and thus the application of the real gas model is justified. More details can be found in [14].

The choice of the mesh to be prepared for simulating the case derives from the considerations reported below (see section 2.4 for further details). In the case of the Cartesian trimmed mesh, a mesh of 14 mln elements have been carried out. The *snappyHexMesh* utility provided with the OpenFOAM package is used. The overall element number is strongly dependent on the required resolution in the gap area. Particularly costly is the resolution of the gap between casing and screw, since an high surface area is involved. The thinner clearance between star wheel and screw is an other area that heavily influences the element number.

2.2. Solver

The solver used in this work must cope with the two main features of the simulation above mentioned: the real gas modelling and the dynamic mesh. Among the set of solvers provided with OpenFOAM, the *rhoPimpleDyMFoam* solver, a compressible transient solver that makes advantage of the Splitting of Operators technique that comes with the PISO algorithm, is suitable for this purpose. Further details regarding the flow solver are reported in [15] and for what concerns details on the moving mesh solver, the reader is referred to [16].

2.3. Real Gas Model

The model presented in this work implements a form of the semi-empirical van der Waals equation of state. Such an equation was proposed by van der Waals as a modification of the ideal gas law, in order to take into account the size

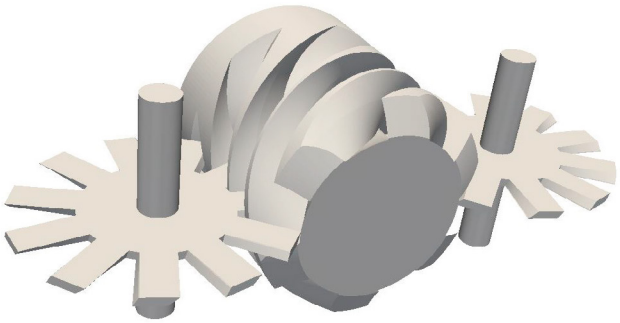


Fig. 1: Rotors of the machine under investigation

of the molecules and the molecular interaction force [17]. This approach overcomes the limits of the ideal gas law in terms of molecular behaviour. Indeed in the ideal gas law molecules are considered as points with perfect elastic collisions. Since actually molecules are not points, attractive and repulsive forces must be kept into account. Indeed, the van der Waals equation of state reported in Eqn. (1)

$$p = p_R + p_A \tag{1}$$

is composed by two terms, the repulsive pressure (in Eqn. (2)),

$$p_R = \frac{RT}{v - b} \tag{2}$$

where b represents a constant related to molecular size and and v is the molar volume. The term $v - b$ is thus related to the reduced specific volume: in other words there is an available volume $v - b$ for each mole for the free motion [18]. An attractive term completes the equation of van der Waals (1).

$$p_A = -\frac{a}{g(v)} \tag{3}$$

Where a is a measure of the intermolecular attraction force.

In the van der Waals model, the two constants a and b together with the real gas constant R define in a unique fashion the properties of the fluid at the critical point. More details can be found in [18]. Such a model suffers of a major drawback: the quantity b is actually variable with pressure and temperature. This fact makes it less reliable at low temperature and high pressure. In order to improve the accuracy in the computation of the density near the critical point, several modification have been proposed in the literature [19]. In this work the one proposed by Peng-Robinson is used.

The Peng-Robinson model requires the properties of the fluid at the critical point and the acentric factor ω. This is because at the critical point the first and the second derivatives of the pressure with respect to the volume vanish [13] and thus expression for a and b can be derived. The acentric factor was proposed as a measure of the amount by which the properties of a substance differ from those predicted by the principle of corresponding states [20]. This principle has been formulated for fluids containing spherical molecules. This kind of fluids correspond to noble gases. Nonetheless, the vast majority of the fluids used in the common practice does not belong to the noble gas category and thus the fluid has non-spherical molecules or molecules with polar groups. If this is the case, systematic deviations in the thermodynamic properties from their spherical counterparts are recorded: these deviations are correlated with the acentric factor. In this framework, this quantity is involved in the definition of the dependence of a from the temperature, and thus it is required for the model set-up. In the following the Peng-Robinson model will be briefly described.

2.3.1. Peng-Robinson

This model is available in both the ESI version OpenFOAM-v1606+ and the extend version. The equation is of the type of Eqn. 1 and its formulation is reported in [13].

$$p = \frac{RT}{v - b} - \frac{a(T)}{v(v - b) + b(v - b)} \tag{4}$$

The formulations for the value of a and b are:

$$a = 0.45724 \frac{\sqrt{RT_c}}{p_c} + \alpha(T_r, \omega) \tag{5}$$

$$b = 0.07780 \frac{RT_c}{p_c} \tag{6}$$

From the former equations, the temperature has effect only on a via the dimensionless function α of the reduced temperature and acentric factor ω. The formulation of α is reported in [13]. The derivation of the density uses the usual formulation reported in Eqn. (7) where the expression for $Z(p, T)$ is reported in [13].

$$\rho = \frac{p}{Z(p, T)RT} \tag{7}$$

2.3.2. Derivation of h,e,s

The quantity relevant for the solution of the energy equation, depending on the formulation h, e, or s, needs to be linked to the temperature. The relation is a user-choice among: constant c_p value, polynomial expression for the temperature dependence, Janaf polynomials or, in the extended version, the NASA equation for the correlation for real gases is available [21]. The polynomial expressions used for the temperature dependence of the specific heat c_p, the viscosity μ and the thermal conductivity κ are taken from the NIST database. The variation of μ and c_p with the temperature is reported in Fig 2.

2.4. Dynamic Mesh Technique

In the following the numerical techniques available within the OpenFOAM framework for the simulation of SSEs are briefly explained. One of the listed technique (i.e. the Key-Frame-Remeshing) will be employed for the simulation and preliminary results are reported in the next section.

2.4.1. Immersed Boundary

The immersed boundary technique, available only within the foam-extend framework, was first proposed by [22] as a numerical method for the simulation of blood flow. Basically it is a method that allows not to conform the mesh to the geometry one needs to simulate, but rather to adapt the flow equations to the geometry. The difficulties are therefore shifted in the inclusion of a source term in the Navier-Stokes equations in the nearby of the boundary. The benefits of this approach increase if one considers the motion of the boundaries, that can cause the degradation of the quality of the conventional body fitted grids [23].

The major drawback of this approach is an higher complexity in the code. In foam-extend 4.0 the immersed boundary method is implemented, as well as the inclusion of the body motion support and turbulence. Nonetheless, no source term for compressible fluids is included. This makes this technique a not rough-and-ready alternative for the simulation of SSEs. The complexity in the coding of boundary conditions for the compressible nature of the fluid involved in this kind of problem makes not straightforward the extension of the available code to compressible cases. Furthermore, being applied on a Cartesian mesh, problems in the resolution of the boundary layer arise. Generally speaking, the boundaries of the geometry are not aligned to the faces of the cell. This is detrimental from the point of view of the boundary layer resolution [23]. This last aspect of this approach is remarkable if thought to be applied to positive displacement machines, where gaps play a crucial role and their behaviour can influence the performance of the machines. A way for resolving this issue is the refinement in the proximity of the boundary. This of course increases dramatically the number of elements. An adaptive refinement technique could be used for overcoming this problem: the refinement is carried out only the areas where the geometric boundaries are. The refinement should therefore follow the motion of the geometry, as reported in [24].

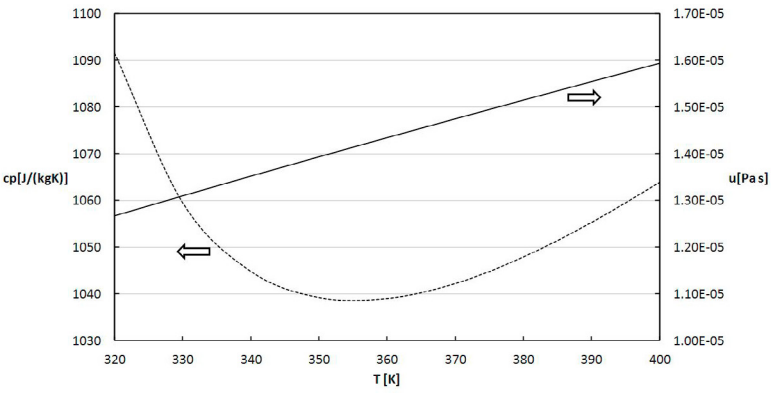


Fig. 2: Variation of thermophysical properties with the temperature. Values for 1 MPa

Summing up, this method could be proficiently used in the design phase, since the meshing time are dramatically reduced, involving only the realization of a Cartesian mesh. For more refined analyses this method is not probably the most suitable one.

2.4.2. Mesh adaption - Dynamic Remeshing

Although only available in the extended version of OpenFOAM, the missing libraries can be easily included even in the OpenFoam-v1606+ suite. This approach is based on an extension of the standard dynamic mesh classes. It is thought for handling simplical meshes (i.e. triangular in 2D and tetrahedral in 3D). It is always used together with mesh smoothing techniques, and the entire re-meshing process can be divided in three steps: mesh smoothing, mesh reconnection and solution remapping.

Mesh Smoothing: by spreading the boundary-induced deformation inside the domain, it continuously maintains the mesh quality. It does not introduce changes in mesh connectivity (called topology changes), and delays local re-meshing requirements. With the class extension it is provided also a wrapper class of the Mesquite optimization library, that overcomes the limits of the usual laplacian smoothing techniques. Classic Laplacian techinque is indeed fast and simple, but easily cells can degenerate. So the Mesquite libraries [25] can alternatively be used: the mesh deformation is associated with the mesh quality. This comes with an higher computational cost, but the technique have been demonstrated to be effective [25].

The second step of the re-meshing algorithm is the adaptive mesh reconnection. This occurs when a cell becomes excessive distorted after the smoothing algorithm has spread the deformation as much as possible inside the domain. In the current state the reconnection is local in order to reduce interpolation errors.

The third and last step of the solver is the remapping of the solution on the new mesh. The procedure involves the creation of a super mesh that comprises both the old local mesh (source) and the new reconnected mesh (target). The steps of the remapping are (i)computation of the intersections between the source and target mesh (ii) the computation and limitation of the gradients on the source mesh (iii) volume and distance weighted Taylor series interpolate to super mesh and finally (iv) the agglomeration on the target mesh.

The major drawback of this approach is that the parallelism has some issues and is not robust. On the top of that, as above mentioned, the Mesquite libraries can handle only simplical cells and thus the only element type allowed is the tetrahedron. Eventually it must be remarked that these libraries are not maintained any longer.

2.4.3. Key Frame Remeshing

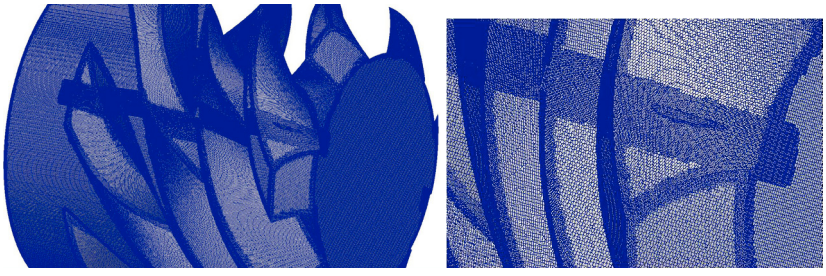
The Key Frame Remeshing Techinque [26] involves the complete re-meshing of the geometry every time the quality of the cells falls below a certain threshold. This tool is basically a wrapper so it is not a package provided with the code itself. The steps are the same pointed out in section 2.4.2, but the re-meshing is total as well as the mapping of the solution. The higher computational time spent for the meshing is compensated by the reliability of parallel consistency. The error in the mass conservation given by the fact that the space conservation law is not observed remains negligible if the overall time simulated is limited. Indeed only a whole revolution of the machine was simulated. This is the approach used in this work. In addition the process can even been speeded up by preparing in advance the set of mesh to be passed to the solver. This could be done while the solver is running but on a different machine or using different nodes. This expedients can reduce the total amount of simulation time and optimise the overall usage of the computational power in case of scalability problems.

This technique have been successfully applied in literature for the simulation of volumetric expanders. Some examples are reported in [26] and [2].

3. Results

The Key Frame technique have been applied to the simulation of the single screw expander. The mesh used for the simulation is the unstructured Cartesian trimmed mesh briefly described in section 2.1. The unstructured mesh is composed by roughly 14 millions elements and allows to achieve an average $y+$ of 20.

Figure 3a reports the particular of one of the mesh used during the calculation. The surface mesh on the screw is reported. As one can see the wall of the screw has an hole: in this area contact happens and thus the mesh of the screw is merged with the star wheel mesh. The resulting contact area is reported in figure 3b. The mesh merging



(a) Mesh of the screw (b) Particular of the screw: contact area

Fig. 3: Overall Mesh and particular of the screw

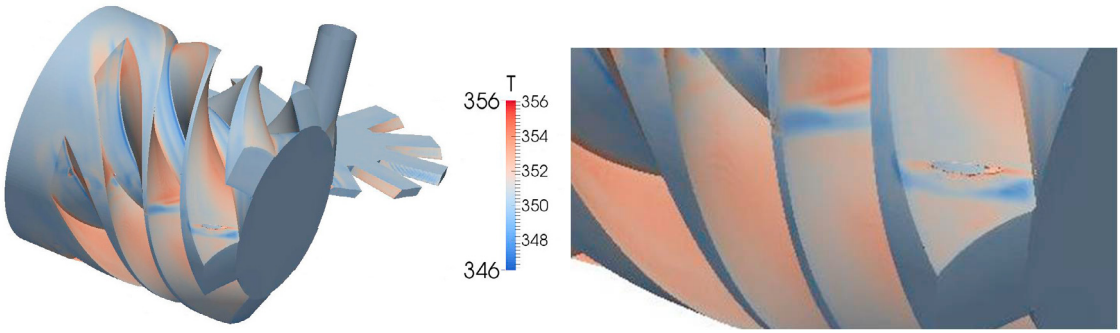
when contact happens is allowed only by using the Key Frame remeshing technique by proper choice of the minimum element size. The *snappyHexMesh* utility will therefore merge two surfaces which are closer than that size and thus the contact between the engaging parts can be kept into account.

The results obtained by the usage of such a technique after the passage of one groove are reported in figure 4. The expansion of the R134a is well represented by the temperature distribution on the flow field. The attention of the reader is driven on the low temperature area downstream the gap. Here the fast expansion of the flow through the gap causes a temperature drop caught by the numerical simulation.

As mentioned in section 2.4.3 the simulations carried out by employing this technique are affected by error in mass conservation due to space conservation law violation. This error propagates as the number of remeshing operation increases. It is thus important to reduce as much as possible these occurrences. In this work, for a SSE rotating at 3000 rpm, the maximum interval of time allowed by the set-up employed by the authors is equal to 10 μs. This value derives from a trial and error procedure. this leads to the employment of roughly 300 meshes per pitch.

4. Conclusion

In this work several numerical techniques able to simulate the complexity of the motion of positive displacement machines have been discussed. The pros and cons of each of the approaches is pointed out and the users can find in this work a review and a reference point of the available methods in the OpenFOAM-v1606+ and foam-extend4.0 framework to simulate such machineries. The necessity for the usage of a real gas model has been discussed as well. Both of the features (dynamic mesh and real gas model) are necessary for the simulation of the flow inside positive displacement machines. Furthermore these aspects of the numerical simulation often represent the most challenging part of the simulation.



(a) Temperature pattern on the screw (b) Temperature pattern downstream the engagement

Fig. 4: Key Frame of Reference results: Temperature pattern on the screw and particular of the engagement area

The Key Frame Remeshing technique was eventually applied for the simulation of a single screw expander. Such a technique is often used in the ORC applications that involves volumetric machineries. This work represents an application of such a technique to overcome the difficulties related to the mesh motion using an open-source software.

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