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Two-phase chamber modeling of a twin-screw expander for Trilateral Flash Cycle applications

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Abstract

Low temperature (<100°C) streams have the largest share of waste heat recovery potential and may represent an attractive opportunity for a sustainable economy. Among the bottoming thermodynamic approaches that have been proposed to convert this waste heat into electricity, the Trilateral Flash Cycle (TFC) proved to be theoretically capable to recover more heat from a low-temperature single-phase heat source than any simple Rankine cycle. However, the commercialization of TFC recovery units has been so far prevented by the lack of an expander technology that should efficiently operate with high mass flow rates of a two-phase flashing flow. A promising candidate to tackle these challenges is the twin-screw technology thanks to its positive displacement nature and the capability to run at high revolution speeds without remarkable efficiency drops.

In the current research work, a twin-screw expander has been modeled in the commercial software GT-SUITE™. The modeling activity resulted in a two-phase chamber model based on the coupling of the conservation equations and the REFPROP library to calculate the thermophysical properties of the liquid-vapor mixture of the R245fa working fluid at each time step. Using pre-processed geometrical data, the model includes a detailed breakdown of the leakage paths and allows to retrieve key information for a future optimization of the machine such as the indicator diagram and the quality-angle diagram. Parametric analyses were eventually carried out to assess the expander behavior at different operating conditions, namely manometric expansion ratio, revolution speed and inlet quality.

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Keywords: Trilateral Flash Cycle; Twin-screw expander; two-phase expander; low grade heat to power conversion

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1. Introduction

Energy recovery is nowadays seen as an attractive opportunity to drive existing state of the art technology towards zero emissions targets. Furthermore, from an economic perspective, significant growth in the waste heat recovery market is projected in the short term future; for instance, in the United States the market size is projected to grow from 44.14 Billion USD in 2015 to 65.87 Billion USD by 2021 [1].

Recent studies state that the theoretical global waste heat potential is 68.2 PWh, the 52% of the primary energy consumptions [2, 3]. This figure refers to the energy that is wasted as exhausts or effluents only (i.e. no radiation or others). In particular, the 63% of the global waste heat potential occurs at temperature levels not higher than 100°C. Therefore, despite the low exergetic content, low grade waste heat recovery might provide undoubtable energetic, environmental and economic benefits in key sectors such as the iron and steel one.

Unlike thermal heat recovery approaches, waste heat to power conversion systems based on bottoming thermodynamic cycles provide an electrical output that can easily be exported even outside the production site. Among the different cycle architectures that have been proposed for waste heat recovery applications, the Trilateral Flash Cycle (TFC) theoretically showed a greater recovery potential from a low-temperature single-phase heat source than any simple Rankine cycle [4].

The principal literature on the TFC are the research works proposed by Ian Smith et al. at City University London that referred to a geothermal low grade heat recovery application [4–6]. In addition, following theoretical works compared the performance of TFC over conventional Organic Rankine Cycles (ORC). In particular, for a heat source at 150 °C and using propane as working fluid, TFC showed an exergy efficiency 30% greater than that of an ORC. Moreover, volume flow rates and, in turn, size of heat exchangers and machines are larger in TFC systems [7]. Water was found to be the best performing working fluid. However, the low saturation pressure at ambient temperature would lead to extraordinarily large volumetric flow rates [8]. The greater exergetic efficiency of TFC over ORC was confirmed by a similar study: in particular, after an analysis of multiple potential working fluids, siloxanes were found to be more suitable both for ORC and TFC applications [9]. Nevertheless, in this study, TFC showed similar energetic performance to ORC due to a throttling valve located in parallel with the expander. An exergo-economic comparison of TFC, ORC and Kalina cycles using a low grade heat source restated that the main advantage of TFC is the good temperature match during the heat recovery and that the TFC power system can be useful if the expander has an isentropic efficiency close to that of conventional turbines; otherwise the ORC is the most advantageous option [10].

The main constraint to the commercial development of TFC system is the two-phase expander. In fact, the presence of liquid phase during the expansion discards turboexpanders. At the same time, those positive displacement technologies that experience severe efficiency drops when high revolution speeds are necessary to match the required large capacities should be also discouraged. For these reasons, twin-screw machines appear to be the most suitable expansion technology. In particular, after several investigations, it was concluded that screw machines may be built no larger than current gas compressors to operate as two-phase expanders [6]. To date, the few experimental activities on twin-screw expanders that have been published employed R113 [6] or water [11]. Maximum measured isentropic efficiency was 70% and 50% respectively.

Twin-screw machine modeling is a research topic widely investigated in the literature. Chamber models [12], where the spatial variation of quantities in the cavity built by male and female rotors lobes is considered homogeneous, as well as three-dimensional computational methodologies [13] have been developed with reference to air and gas compressors [12], and for single phase ORC expander applications [14]. Two-phase twin-screw expanders have been also modeled with a lumped parameter approach in [6] and [15]. In both the studies, mass and energy equations were coupled with customized subroutines for the calculation of local thermodynamic and transport properties of the liquid-vapor mixture working fluids [5] while leakage flows were modeled as orifices.

In the current paper, a twin-screw expander for low grade heat to power conversion based on a Trilateral Flash Cycle was modeled in the commercial environment GT-SUITE™ [16]. The novel features of this approach lie in the calculation of thermodynamic properties of the working fluid relying on the NIST REFPROP database [17], in the possibility to predict pressure pulsations at the intake and exhaust, and in the detailed leakage breakdown. After introducing the modeling methodology, a sample test case is presented and its pressure-Volume and quality-angle diagrams discussed. Parametric analysis at different operating conditions were eventually carried out to assess the thermodynamic capabilities of the expander at model level.

2. Modelling Approach

GT-SUITE™, the commercial software environment in which the twin screw expander model has been developed, is based on a one-dimensional formulation of Navier-Stokes equations and on a staggered grid spatial discretization. According to this approach, each system is discretized into a series of capacities such that manifolds are represented by single volumes while pipes are divided into one or more volumes. These volumes are eventually connected by boundaries. The scalar variables (pressure, temperature, density, internal energy, enthalpy, etc.) are assumed to be uniform in each volume. On the other hand, vector variables (mass flux, velocity, mass fraction fluxes, etc.) are calculated for each boundary [16, 18].

The schematic of the TFC expander model, which applies to any positive displacement machine, is reported in Figure 1. Once discretized, in the inlet and outlet pipes the scalar equations (mass, energy) are solved at the centers of finite volumes, and the vector (mass flow) at the boundaries between them. The intake and exhaust manifolds are modeled as capacities of finite volume and connect the pipes with the filling and emptying expander cells respectively. These components are named “flowsplits” and have multiple openings whose number depends on the number of cells and of the leakage paths. The solution of the flowsplit is similar to the pipe: the scalars are solved at the center of the volume, while the solution of the momentum equation is carried out separately at each of the volume openings (boundaries). The expander cells, that are physically generated when male and female rotor lobes engage, are treated as capacities with uniform properties and whose volume varies according to a law that is given as input of the calculation since the software does not provide a geometrical pre-processor yet. In addition to the revolution speed, inlet and outlet boundary conditions, which physically would be respectively provided by the heater and the receiver of the TFC system, in this standalone model of the expander have been considered as plenums of infinite capacity.

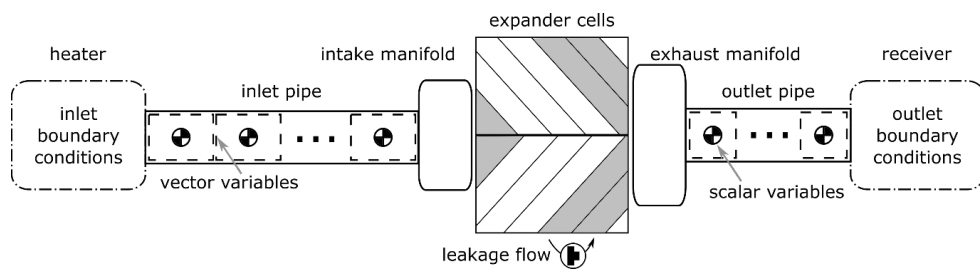


Fig. 1. Modelling scheme

Similarly to any chamber modelling approach, leakages are herein considered as flow through an orifice. In particular, the incompressible Bernoulli equation is used for liquids while the isentropic nozzle relationships for subsonic and supersonic regimes are considered for gases and require the calculation of the ratio of specific heats (γ). Two-phase leakage flows are calculated using the formulations valid for gases and assuming an equivalent γ as the weighted average, based on quality, of the ratio of specific heats for thermodynamic states at saturated conditions, as per Equation (1).

$$\gamma_{eq} = \gamma_{vap} x + \gamma_{liq} (1 - x) \quad (1)$$

Other literature studies model the leakage through an orifice assuming as isenthalpic process whereas the leakage fluid is at the same thermodynamic conditions of the high pressure region [19]. This approach involves the calculation of the dynamic viscosity (μ) of the two-phase fluid based on the quality (x) and computed according to Equation (2).

$$1/\mu_{eq} = x/\mu_{vap} + (1 - x)/\mu_{liq} \quad (2)$$

Assuming adiabatic conditions for pipes and expander cells and neglecting the influence of potential energy variations, the conservation equations are solved through an explicit 5th order Runge-Kutta integration scheme whose primary solution variables are mass flow rate, density, and internal energy. In particular, to calculate mass and energy in a given volume at the following time step (that needs to satisfy the Courant condition for numerical stability), continuity and energy equations are firstly used and involve the reference volume and its neighbors. With the volume and mass known, the density is calculated yielding density and energy. Using a dynamic-link library (DLL) of the

NIST REFPROP database [17] embedded in the software package, the solver iterates on pressure and temperature until they satisfy the density and energy already calculated for this time step.

3. Simulation setup

The software environment GT-SUITE™ does not yet provide a template for screw machine analysis. Hence, a customized model had to be developed for the two-phase twin-screw expander whose main features are reported in Table 1.

Table 1. Main geometrical and operating features of the expander

Rotor Diameter	127 mm	Suction / Discharge ports arrangement	axial / axial
Aspect Ratio (L/D)	1.65	Revolution speed range	1500-6000 RPM
Built-in Volume ratio	5	Tip speed range	10.01-40.06 m/s
Male / Female rotor lobes	4/6	Weight	220 kg

A fundamental input for the model setup were the geometrical features of the machine which were provided by the industrial manufacturer. This information included angular evolution of cell volume, suction and discharge areas as well as the main leakage paths. The first three quantities are displayed in Figure 2 over an angular period whose extent depends on geometrical features of the machine such as male/female rotor lobes and wrap angle (873° in the investigated machine). As concerns the leakage paths, six different categories were identified according to the literature [20] and reported in Figure 3. Equivalent orifices with the same colors modeled the corresponding leakages paths in the model block diagram displayed in Figure 4. The information about leakages were expressed in terms of equivalent area of the leakage passage. The effects of thermal deformation on clearances have been not considered.

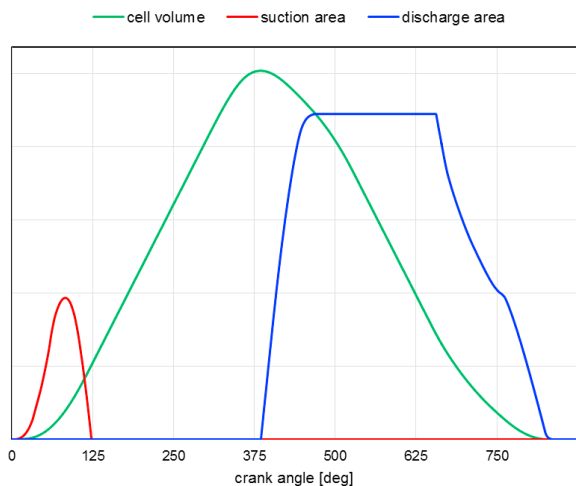


Fig. 2. Angular evolution of expander cell volume and interaction with suction and discharge ports

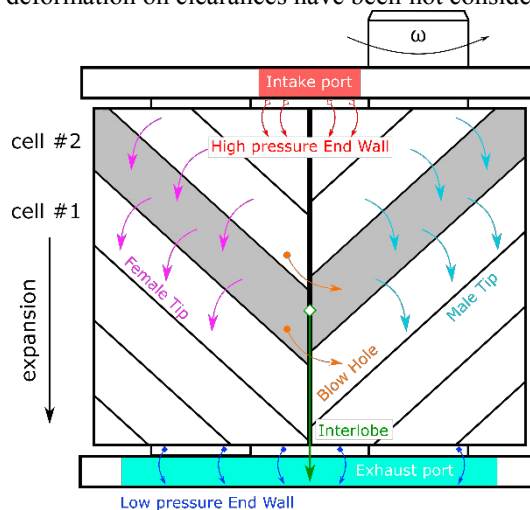


Fig. 3. Leakage paths in a twin-screw expander (elaboration from [20])

The modeled geometry of the machine is shown in Figure 4. The expander inlet is composed of two suction lines fed by the same boundary conditions, namely pressure and inlet quality that a real TFC expander would see after the heat recovery process. The two feeding lines merge in the intake volume where the working fluid is made available to the expander cells during the suction phase. During suction, part of the expansion process takes place since the volume of the intake manifold is larger than those of the pipes to ensure a correct filling of the expander cells. However, this expansion does not produce any work. Similarly, after the closed-volume expansion phase, the contributions from the different cells merge in the exhaust manifold and eventually go towards the receiver and then to the condenser through the outlet pipe. Hence, additional boundary conditions are the condensation pressure and the

expander revolution speed. However, since the angular cycle duration was greater than 360° or 720° (the only values accepted by the software), the angles (but not the magnitudes) of all the geometrical inputs and the revolution speed had to be scaled. For instance, with reference to the current study, the scaling factor for the geometrical quantities and the revolution speed was 2.425 ($873^\circ/360^\circ$). In this way, the mass flow rate calculated in a simulation cycle corresponds to the mass flow rate of the actual operating cycle.

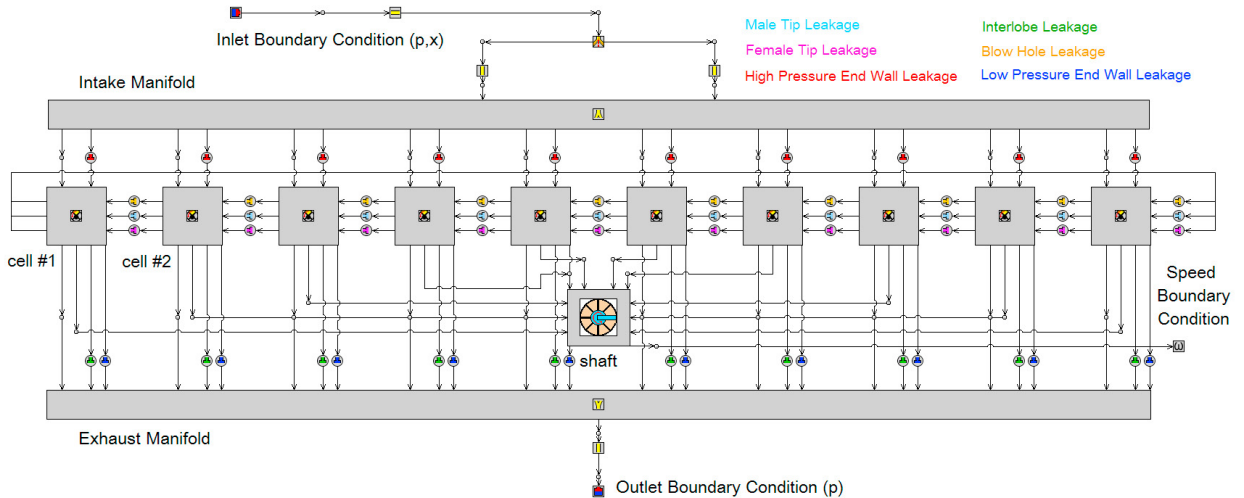


Fig. 4. Twin-screw expander model diagram in GT-SUITE™

4. Results and discussion

4.1. Test case

With reference to the operating conditions listed in Table 2 and R245fa as working fluid, Figures 5 and 6 report the indicator (p - V) diagram and the angular evolution of fluid quality respectively.

Table 2. Simulation variables

	Inlet pressure	Inlet quality	Revolution speed	Outlet pressure
Test case (Figures 5 and 6)	8 bar _a	0.11	4070 RPM	1.3 bar _a
Parametric analysis (Figures 7 and 8)	3-10 bar _a	0.0-0.4	1500-6000 RPM	1.3 bar _a

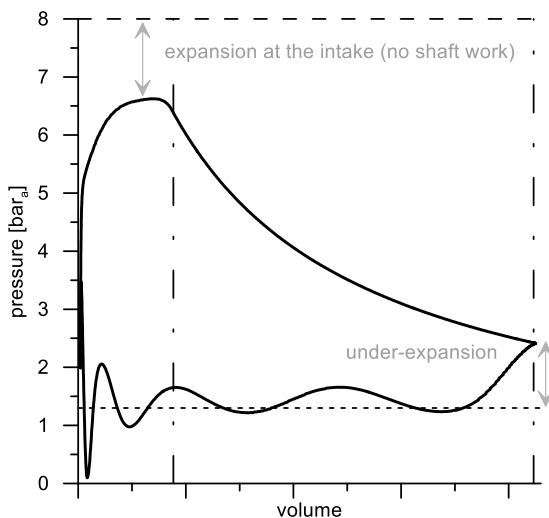


Fig. 5. Indicator diagram

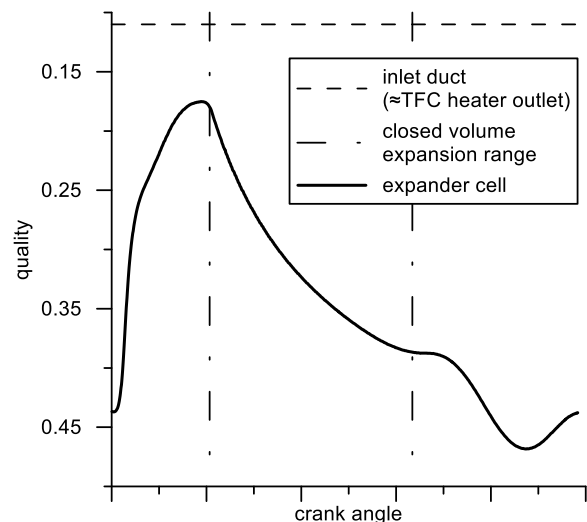


Fig. 6. Angular quality evolution

Due to the expansion at the intake manifold and to the pressure losses from the inlet boundary conditions to the actual suction process of the expander cells, 1.5 bar pressure drop and an inlet quality of 0.17 instead of 0.11 can be noticed. In the closed volume expansion process, the cell pressure drops to 2.5 bar while the quality reaches 0.40. However, due to the mismatching of the built-in volume ratio of the expander to the pressure ratio imposed, a sudden expansion can be noticed. In turn, the quality drops to 0.45 while pressure pulsations at the discharge with an amplitude of nearly 0.5 bar can be noticed.

During the intake process, screw expanders tend to show pressure oscillations that however the model does not predict. This fact is likely due to the type of boundary conditions set at the inlet that, unlike the ones at the outlet, could not be set as an open boundary. Therefore, any backflow, which would have triggered pressure pulsations is suppressed. Nonetheless, this assumption will be overcome when the expander model will be connected to the overall TFC system, whose modeling activity is ongoing.

As concerns the pressure pulsations at the beginning of the exhaust phase, they result from the dynamic phenomena that occur between the emptying expander cell and the exhaust line, which is at a lower pressure. The amplitude of the pulsation is proportional to the magnitude of the under-expansion and, in turn, to the mismatching between the built-in and manometric pressure ratios. On the other hand, towards the end of the cycle, higher pressure peaks are calculated. These effects, which might not happen in real machines, depend on the geometrical input quantities. As can be noticed from Figure 2, there is an angular phase in which the cell volume and the discharge port area both decrease towards values theoretically close to zero. In this range, a small decrease in volume triggers high pressure in the cell despite the presence of the leakage gaps. Furthermore, from a numerical viewpoint, this phenomenon complicates the convergence of the solution and forces the numerical method to use lower time steps. Since the volume in this angular range is very low, the impact of these unexpected pressure peaks on the overall indicated power is limited. Nonetheless, in future releases of the expander model, manufacturing and mounting tolerances will be taken into account to correct the geometrical input quantities and minimize this issue.

4.2. Parametric analysis

A further design exploration was performed with reference to the operating conditions in Table 3. In particular, Figures 7 and 8 report the performance trends that could be achieved at the operating conditions of Figures 4 and 5 but varying two variables per time.

As shown in Figure 7.a, high pressures and low qualities at the inlet of the expander contribute, for a given revolution speed, to increase the mass flow rate since they both affect the fluid density. Another parameter that is directly related to the mass flow rate is the expander revolution speed. In Figure 8.a one can notice a trend that conflicts with the theoretical proportionality between mass flow rate and revolution speed. In fact, above a certain threshold, mass flow rate does not increase with revolution speed anymore. This fact is due to the magnitude of the expansion process that occurs from the inlet section to the actual suction port of the machine, similarly to what is shown in Figure 5. In particular, high revolution speeds enhance this expansion and lead to a lower suction pressure as well as to a greater quality. Depending on this phenomenon, the under-expansion shown in Figure 5 can be reduced as presented in Figure 9.a, or even lead to an over-expansion. Since the density at the suction port is lower than the one at the inlet, the expander volumetric efficiency (η_{vol}) decreases. This parameter is a result of the calculation and it is defined as the ratio of the actual mass flow rate measured at the outlet pipe (m_{out}) and the theoretical value which depends on density (ρ) and cell volume (V) at the end of the suction process as well as on the number of cells (Z) and the revolution speed (ω) expressed in RPM (Equation (3)).

$$\eta_{vol} = m_{out} / \left(\rho_{suc} V_{suc} Z \frac{\omega}{60} \right) \quad (3)$$

The mass flow rate stagnation at high revolution speeds additionally affects the indicated power. This quantity is defined as the area of the indicator diagram of the single cell multiplied by the cell frequency (Equation (4)).

$$P_{ind} = Z \frac{\omega}{60} \oint p dV \quad (4)$$

Indeed, despite the proportionality relationship between revolution speed and indicated power, the reduction of suction pressure at high revolution speeds impacts on the area of the indicator diagram shown in Figure 5 and, in turn, on the overall indicated power. On the other hand, for a given revolution speed, an increase of the inlet pressure always results in a greater indicated power, as shown in Figures 7.b and 8.b. The motivations for this increase are twofold: on one hand there is the greater expansion ratio while on the other one there are effects on the mass flow rate which have been previously described. As concerns the effects of inlet quality on indicated power shown in Figure 7.b, the greater the quality, the lower is the mass flow rate as well as the indicated power. In fact, as reported in Figure 9.b, for the same pressure ratio the nature of the closed volume expansion phase completely changes depending on the inlet quality.

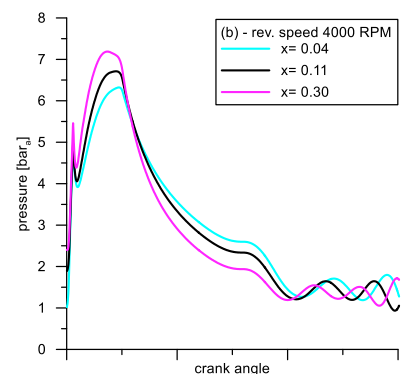
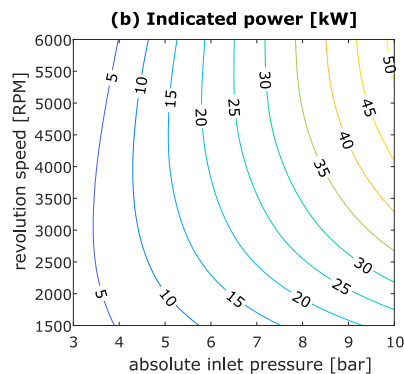
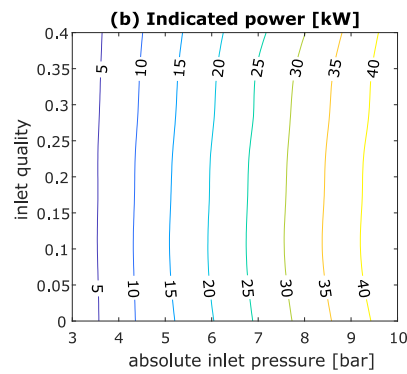
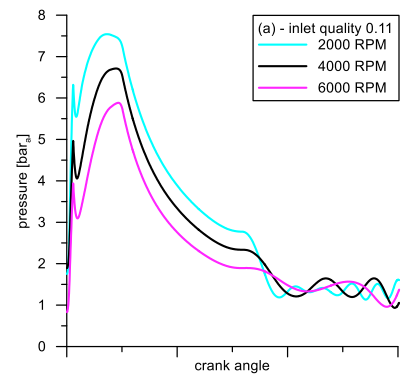
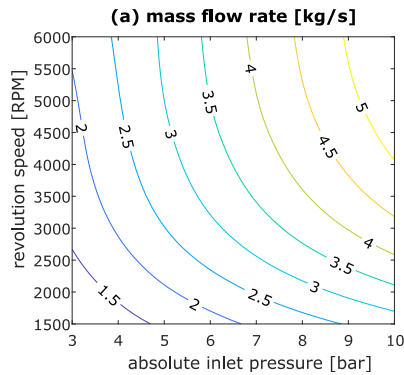
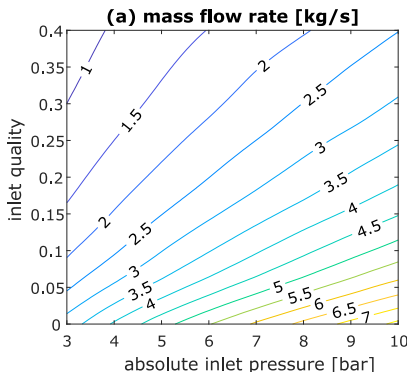


Fig. 7. Performance maps (revolution speed 4070 RPM)

Fig. 8. Performance maps (inlet quality 0.11)

Fig. 9. Pressure-angle diagrams (inlet pressure 8 bar_a)

5. Conclusions

In this research work the fluid dynamic performance of a twin-screw expander have been investigated with reference to a Trilateral Flash Cycle applications for low grade heat to power conversion. The numerical methodology that was employed led to the development of a chamber model of the expander in the commercial software environment GT-SUITE™. Although spatial variation of thermodynamic quantities in the machine cannot be appreciated, this approach allows to outline and optimize design configurations with the development times of the one-dimensional computational fluid dynamics.

To setup the model, geometrical data regarding cell volume evolution, suction and discharge port areas as well as leakage area in the different paths of a twin-screw machine are fundamental. In this specific case these quantities were provided by the expander manufacturer but they could also be generated using commercial software tools specifically for twin screw machines, literature models or 3D CAD drawings.

The model was tested with reference to a TFC application with a manometric pressure ratio of 6.15 and an inlet quality of 0.11. The pre-expansion at the intake manifold and the under-expansion due to the mismatching of the manometric pressure ratio with the built-in volume ratio of the expander (equal to 5) were some of the phenomena

that could be appreciated through the modeling platform. Accurate modeling of leakage flows and predictions of pressure pulsations need more development. Further parametric analysis investigated the effect of inlet conditions and revolution speed on the expander performance in terms of indicated power and mass flow rate. In the reference test case these quantities were equal to 4.2 kg/s and 32.7 kW respectively.

Due to the simplified nature of the model and the assumptions made (e.g. two-phase mixture as an equivalent gas), future studies will aim at comparing this approach with more advanced ones (3D CFD) but mainly through a detailed experimental campaign on a TFC test bench. Indeed, a severe limitation that the model at the state of the art has is the incapability of predicting friction losses that would provide insights on the overall expander efficiency in the TFC field. Nonetheless, even without friction modelling numerical and experimental indicator diagrams can be compared.

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