DYNAMIC MODEL FOR THE PERFORMANCE PREDICTION OF A TWIN SCREW EXPANDER IN AN ORC

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ABSTRACT

The Organic Rankine Cycle (ORC) is well known and proven technology for waste heat recovery. The current generation of twin screw expanders used for low-grade heat recovery are in fact compressors working in the opposite sense. In this paper a mathematical model for calculating the performance of a twin screw expander is presented. The model is based on geometrical parameters which describe volume and leakage areas for every angular position. With these functions the entire design of a screw expander is determined. The differential equations used in the model are derived from the mass and energy conservation laws and are solved together with the appropriate Equation of State in the instantaneous control volumes. Since R245fa is selected as a working fluid, the Aungier Redlich-Kwong Equation of State has been used. The results of the mathematical model are compared to the 3D Computational Fluid Dynamics (CFD) calculations of the same twin screw expander using the same working fluid. To calculate the mass flow rates through the leakage paths formed inside the screw expander, flow coefficients are considered as constant and they are derived from 3D CFD calculations. The outcome of the mathematical model is the P-V indicator diagram which is compared to CFD results of the same twin screw expander. It is shown that the developed model accurately predicts the performance of the expander.

1. INTRODUCTION

With increasing concerns over energy pollution and consumption constraints the interest in waste heat recovery has grown in the past years. A large portion of waste heat is available at low temperatures (350K-400K) from industrial processes which can be converted into mechanical power. The most widely used technology for waste heat recovery is the Organic Rankine Cycle (ORC). Although ORC systems are now well developed, efforts have been increasingly directed towards higher efficiencies and power outputs. The key element for the power generation in ORC systems is the expander. The choice of the expander is crucial and it depends on the amount of available heat and operating conditions. For small scale ORC system studied in this paper, displacement machines are highly suitable (Lemort, 2013).

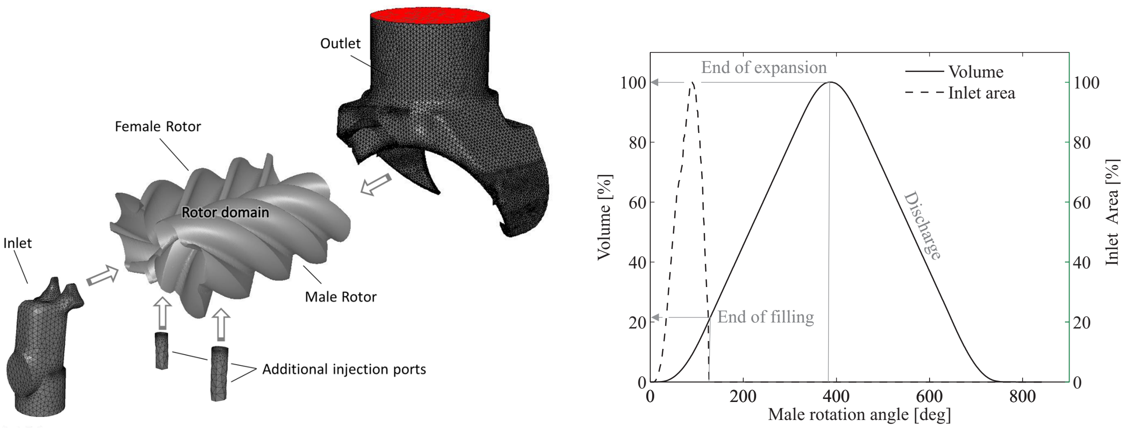
The first analytical procedure for the expander's performance prediction has been reported by (Margolis, 1978). More recently, the numerical and experimental study of an oil injected twin screw expander for both air and R113 has been presented in (Wang, 2010). A mathematical model was verified with an experimental study and flow coefficients used in the leakage models were derived from it.

The capability to analyse the performance of such complex screw machines by thermodynamic models which describe the behaviour of the fluid are often limited because of inability to get proper experimental data. With Computational Fluid Dynamic (CFD) it is possible to analyse the flow within screw expanders and to get a better view on different phenomena that occur within such machines. In previous studies the authors presented a 3D CFD simulation of a twin screw expander using R245fa (also known as 1,1,1,3,3-Pentafluoropropane) as the working fluid (Papes, 2014). R245fa is characterized by a positive slope of the saturated vapor line in a T-s diagram which will prevent the formation of liquid droplets at the exit of the expander. The mesh motion is handled by an in-house code which generates a block-structured grid with the help of solutions of Laplace problems on an unstructured triangular grid (Vande Voorde, 2004).

The aim of this paper is to present a mathematical model of a twin screw expander and to validate it with CFD results. Moreover, the goal is to extract the coefficients used in the isentropic converging nozzle leakage model from the 3D CFD analysis. Several objective performance indicators such as mass flow rates, pressure-volume diagrams and power output are used to compare these two models.

2. GEOMETRY

The geometry of a twin screw expander used in this study is shown in Figure 1a. There are four male lobes and six female lobes with asymmetrical rotor profiles. The outer diameter of the male and female rotors is approximately $70mm$ with L/D ratio of 1.9.



(a) Geometry **(b) Volume of the chamber**

Figure 1: Geometry of a twin screw expander with the analytical description of the geometrical parameters used in the mathematical model

The volume curve of the screw expander is shown in Figure 1b. The formation of a chamber starts at $\theta = 0°$ in Figure 1b. When $\theta = 7°$, the chamber is in connection with the inlet port. As the rotor rotate, the volume of the chamber increases with increasing inlet surface area, and the chamber is filled with the working fluid. When the inlet area starts to decrease, the volume of the chamber is still increasing. This can already cause the **pre-expansion** of the working fluid. The filling ends at $\theta = 126°$ after which the working fluid expands with increasing volume of the chamber. At $\theta = 387°$, the working chamber is connected to the outlet and the working fluid is discharged through the outlet port.

Within twin screw expanders, it is possible to identify four types of leakage paths. All four types of leakages in screw expanders are depicted in Figure 2 and are characterized by the length of the leakage path and the area of the clearance.

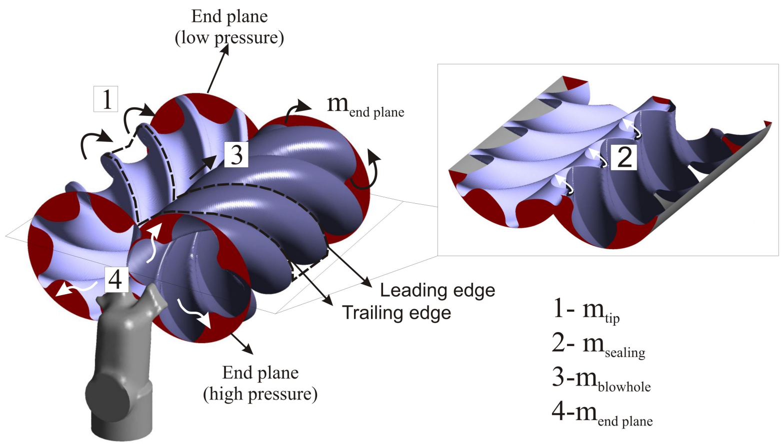


Figure 2: Different leakage types inside the twin screw expander

3. CFD ANALYSIS

The flow calculations inside a screw expander are performed by Ansys Fluent with the use of User Defined Functions (UDFs) to handle the grid movement and real gas model as presented in (Papes, 2014). The mathematical model consists of a set of momentum, energy and mass conservation equations, which are accompanied by the Aungier Redlich-Kwong (ARK) EoS and $k - \varepsilon$ turbulence model. The spatial discretization is second order upwind. Both CFD and mathematical model presented in this paper used the same geometry from Figure 1b. A result of the CFD analysis for pressure ratio of 6 is presented in Figure 3.

In order to calculate flow coefficients for different leakage paths, the mass flow rate through the corresponding leakage path was correlated with the pressure ratio between chambers that are forming that leakage path and its area according to equation of isentropic converging nozzle.

By analysing the results of CFD calculations, it was seen that pulsations in the inlet pipe play an important role in the pressure difference which influences the mass flow during the filling. These pulsations can be captured with 3D CFD calculations or with a one-dimensional model. In this study pulsations in the pipe before the inlet port are obtained from the CFD results and are used in the developed mathematical model. The results of pressure pulsations for different

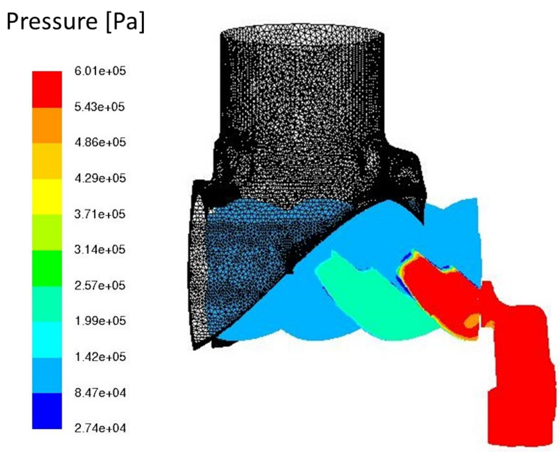


Figure 3: Pressure within twin screw expander (results of CFD analysis)

pressure ratios and rotational speeds were calculated through the reference plane as shown in Figure 4.

4. EQUATIONS GOVERNING SCREW EXPANDER PROCESS

The zero-dimensional mathematical model described in this paper employs the mass and energy conservation equations, accompanied by the geometrical model which describes the change in volume with the time or angular position, as well as change in the inlet and leakage path areas. Also in this model, the ARK EoS is used to describe real gas effects of R245fa.

When analysing the flow within the screw expander, the following assumptions have been made:

- The heat transfer between the working fluid and the rotor or between the casing and the ambient are not included in the model (they are also neglected in CFD simulations).
- Mechanical losses of the screw expander are not included in the model.
- Potential and kinetic energy of the working fluid are negligible.
- The flow through the leakage paths and inlet port is assumed to pass through an isentropic nozzle.
- Leakage flows through the end planes are not included in the model since they are not modelled. in the CFD calculations.
- The discharge process occurs at constant pressure.

The following equations were applied for each working chamber:

$$\frac{dm_{ch}}{dt} = \sum_i \dot{m}_i \tag{1}$$

$$\frac{dT}{dt} = \frac{-T\left(\frac{\partial\rho}{\partial T}\right)_v \left[\frac{dV}{dt} - v\frac{dm_{ch}}{dt}\right] - h\frac{dm_{ch}}{dt} + \sum_i \dot{m}_i h}{m_{ch}c_v} \tag{2}$$

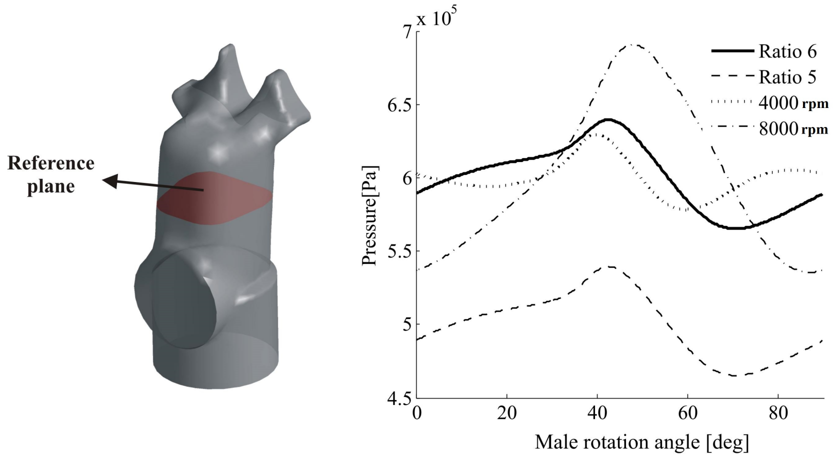


Figure 4: Pressure pulsations in the reference plane of the inlet port (results from CFD analysis)

This system of differential equations is solved by using the forward Euler method applied simultaneously on all chambers. Once the geometrical inputs (volume change and leakage areas) have been provided to the model, the pressure and the temperature are initialized with guess values. After that, for each iteration step, the mass flows going in or out of the chamber are calculated and the temperature in the next step is obtained. Since the mass, the volume and the temperature are then known, the pressure and the density can be updated.

The mass flow through the leakage paths and the inlet port is calculated using the isentropic nozzle model (Bell, 2011):

$$\dot{m}_{nozzle} = CA\sqrt{p_{up}\rho_{up}}\sqrt{\frac{2k}{k-1}\left(p_{ratio}^{2/k} - p_{ratio}^{(k+1)/k}\right)} \tag{3}$$

Where the function of pressure ratio is defined as:

$$p_{ratio} = \begin{cases} \left(1+\dfrac{k-1}{2}\right)^{k/(1-k)} & p_{down}/p_{up} \leq \left(1+\dfrac{(k-1)}{2}\right)^{k/(1-k)} \\ p_{down}/p_{up} & p_{down}/p_{up} > \left(1+\dfrac{(k-1)}{2}\right)^{k/(1-k)} \end{cases}$$

Flow coefficients C are constant in time and are obtained from CFD calculations. The indicated work of a twin screw expander can be expressed as the area of the P-V indicator:

$$W_{ind,cycle} = \int_{cycle} V dp \tag{4}$$

The power of the twin screw expander can be then calculated as:

$$P_{ind} = \frac{W_{ind,cycle} z n}{60} \tag{5}$$

with z the number of lobes and n the rotational speed.

5. RESULTS AND DISCUSSION

There are different parameters to be compared between the developed mathematical model and the CFD analysis. One is the P-V indicator diagram of the screw expander, which will show how the pressure in every moment is changing with the instantaneous volume. If the calculated P-V indicator diagram agrees with the results of CFD analysis, the overall performance will be well predicted. However, additional parameters like mass in the chamber or leakage flow through the clearance paths should be checked and compared.

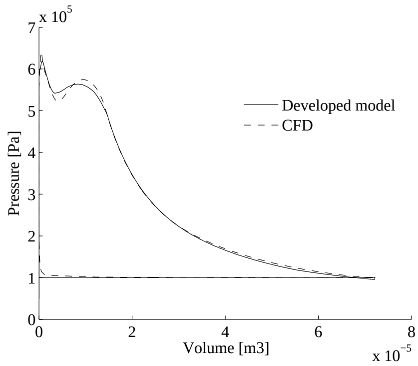
In Table 1, comparison for power and mass flow rate between the developed model and the CFD analysis are presented. The comparison has been made for pressure ratios $\pi = 6, 5$ and 4 and for rotational speeds of $6000rpm$ (nominal speed), $4000rpm$ and $8000rpm$.

5.1 Evaluation with different pressure ratio

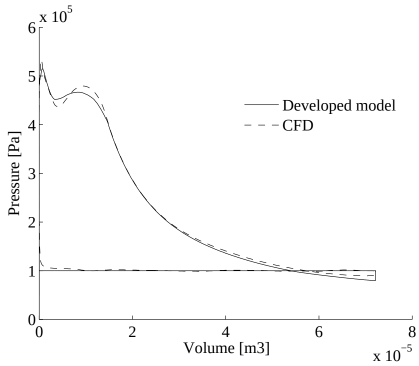
In Figure 5 the P-V indicator diagrams for pressure ratio of $\pi = 6, 5$ and 4 are shown. From Table 1 it can be seen that the difference in power outputs between CFD analysis and developed model is from $2 - 6\%$.

Pressure ratio	Speed	CFD		MODEL	
		Flow rate [kg/s]	Power [kW]	Flow rate [kg/s]	Power [kW]
6	6000	0.1469	4.72	0.1415	4.61
5	6000	0.1210	3.46	0.1160	3.30
4	6000	0.0955	2.18	0.0922	2.05
6	4000	0.1055	3.18	0.1028	3.23
6	8000	0.1618	5.11	0.1619	5.30

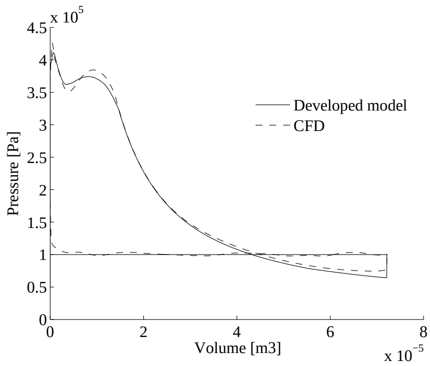
Table 1: Results for mass flow rates and power outputs for the developed model and the CFD analysis



(a) Pressure ratio 6



(b) Pressure ratio 5



(c) Pressure ratio 4

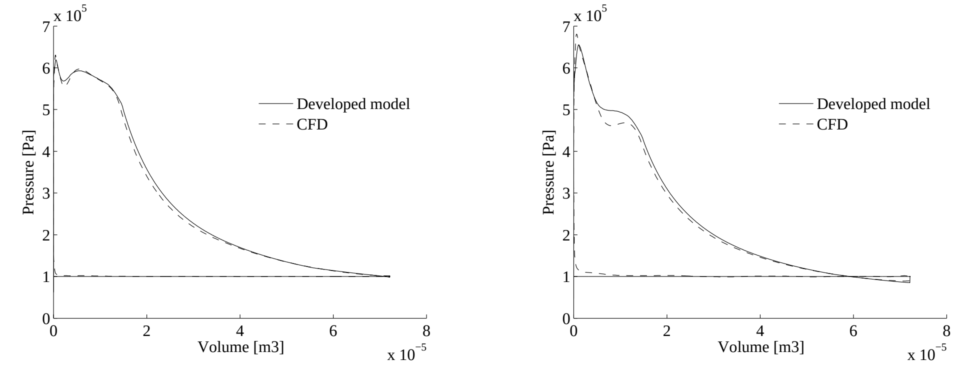
Figure 5: Model predicted and CFD calculated results

5.2 Evaluation with speed change

The performance of the expander was also examined with variations in speed (Figure 6). With change in speed, the P-V indicator shows a difference during the filling phase. Due to the shorter duration of the filling period with the rise in rotational speed, it can be seen that the throttling loss increases. The difference between the developed model and the CFD analysis is around 4% for a rotational speed of 8000rpm and around 2% for a rotational speed of 4000rpm.

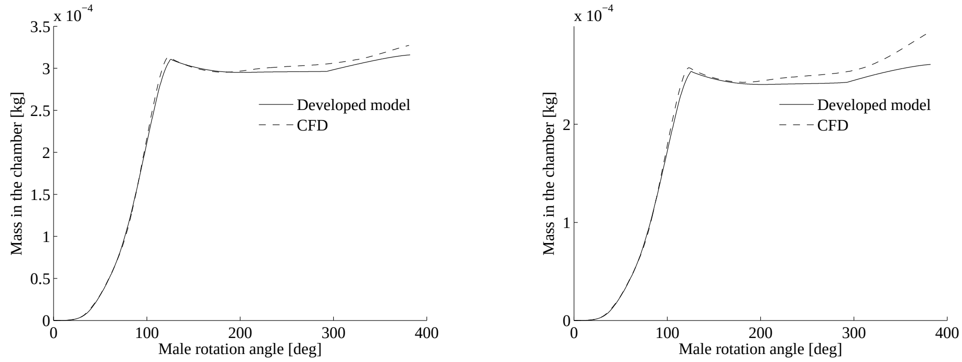
5.3 Mass in the chamber

The comparison of the total mass in the chamber between the developed model and the CFD results is shown in Figure 7. This parameter is very important because it shows if the mass in the chamber after the filling is close to CFD results. This shows if the filling process in the developed model is described correctly. But also, it shows if the leakage flows are reducing the mass in the chamber in the same way as in CFD results.

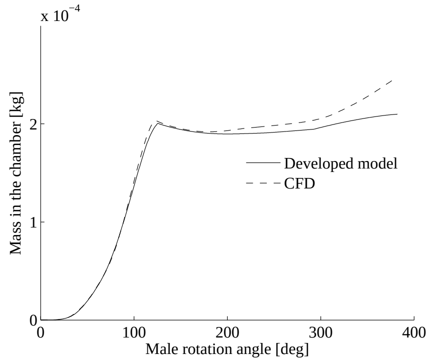


(a) 4000rpm **(b) 8000rpm**

Figure 6: Model predicted and CFD calculated results for changes in rotational speed



(a) Pressure ratio 6 **(b) Pressure ratio 5**

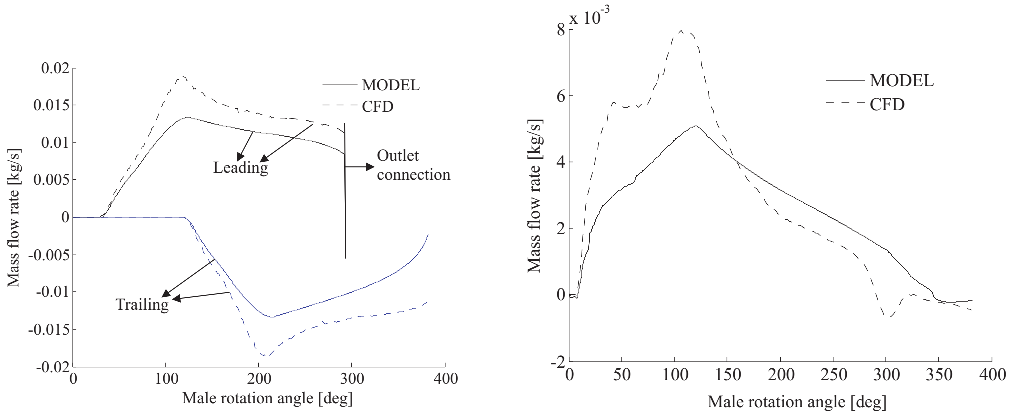


(c) Pressure ratio 4

Figure 7: Model predicted and CFD calculated results of the mass in a chamber for changes in pressure ratio

5.4 Leakage flows

The last two parameters are the mass flow rates through the tip and sealing leakage path (Figure 8). Here it is very important to see if using the constant flow coefficient derived from the CFD calculations can estimate these flows correctly. It can be clearly seen that the trend of these curves is matching well with CFD results. Although slight deviations are present, it should be noted that mass flow rates through the leakage gaps are already very low comparing to the total mass flow rate.



(a) Tip Leakages **(b) Sealing leakage**

Figure 8: Model predicted and CFD calculated results in the screw expander with pressure ratio 6 and rotational speed of 6000rpm

6. CONCLUSION

A mathematical model for the performance prediction of a twin screw expander has been developed. From the mass and energy conservation laws, differential equations are derived which are then solved together with the Aungier Redlich-Kwong Equation of State for R245fa in the instantaneous control volumes. The mathematical model employs all geometrical parameters such as chamber volume, suction and leakage areas. To calculate the mass flow rates through the leakage paths formed inside the screw expander, flow coefficients are derived from CFD analysis. All geometrical inputs in terms of rotational angle of male rotor are employed in the model. It is shown that the developed model accurately predicts the performance of the expander.

7. NOMENCLATURE

NOMENCLATURE

Symbols

$\dot{m}$	Mass flow rate (kg/s)
ρ	Density (kg/m^3)
A	Area of the leakage path/inlet area (m^2)
C	Flow coefficient $(-)$
h	Specific enthalpy (kJ/kg)
k	Specific heat ratio $(-)$
m	Mass (kg)
n	Rotational speed (rpm)
P	Power (W)
T	Temperature (K)
V	Volume (m^3)
W	Work (J)
z	Number of lobes $(-)$

Subscripts

ch	Chamber
$down$	Downstream
i	Number of boundaries of the working chamber
in	Indicated
up	Upstream

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