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Numerical simulation of a twin screw expander for performance prediction

Iva Papes,Joris Degroote,Jan Vierendeels

Department of Flow, Heat and Combustion Mechanics,Ghent University, Belgium

E-mail: iva.papes@ugent.be

Abstract.
With the increasing use of twin screw expanders in waste heat recovery applications, the performance prediction of these machines plays an important role. This paper presents a mathematical model for calculating the performance of a twin screw expander. From the mass and energy conservation laws, differential equations are derived which are then solved together with the appropriate Equation of State in the instantaneous control volumes. Different flow processes that occur inside the screw expander such as filling (accompanied by a substantial pressure loss) and leakage flows through the clearances are accounted for in the model. The mathematical model employs all geometrical parameters such as chamber volume, suction and leakage areas. With R245fa as working fluid, the Aungier Redlich-Kwong Equation of State has been used in order to include real gas effects. 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 Computational Fluid Dynamic calculations at given working conditions and applied to all other working conditions. The outcome of the mathematical model is the P-V indicator diagram which is compared to CFD results of the same twin screw expander. Since CFD calculations require significant computational time, developed mathematical model can be used for the faster performance prediction .

1. Introduction

For more than half a century, screw machines have extensively been used as compressors. In recent years, screw machines as expanders play an important role in waste heat recovery applications. One of the leading technologies in these applications is the Organic Rankine Cycle (ORC). Low-grade enthalpy should be converted to useful work in ORC systems. Given its power range, efficiency and price, the twin screw expander is highly suitable [1]. The optimization of a screw expander's performance can be covered from different points of view such as efficiency, power output, cost, noise and vibrations, etc.

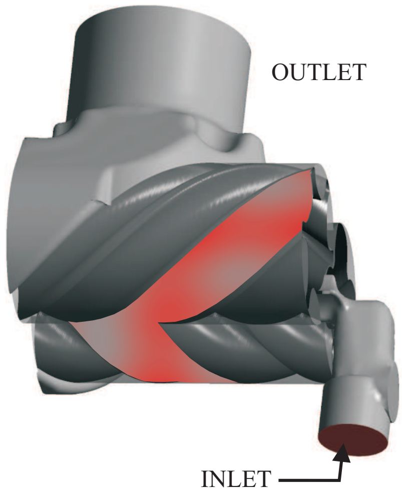
Analytical procedures for the compressors performance prediction have been extensively reported by numerous authors among which Stosic, Fleming, Fujiwara and Hanjalic contributed [2, 3, 4, 5]. Surprisingly, only few publications on the analysis of screw expanders can be found in the literature. The first analytical model for dry screw expanders was presented in [6]. More recently, the numerical and experimental study of an oil injected twin screw expander for both air and R113 has been presented in [7]. The mathematical model was verified with the experimental study and flow coefficients used in the leakage models were evaluated as constant. However, the limitation of the experiments is that they cannot accurately measure flow properties in the clearance area or during the filling. As it is shown in [8], with CFD calculations it is possible to overcome these limits. Therefore, in this model results of the 3D CFD analysis are used in order to better predict the leakage flows and pressure drop during the filling.

Modelling of the leakage flows presents an important and one of the most challenging parts of mentioned mathematical models. A typical leakage model used when modelling scroll or screw types positive displacement machines, is the isentropic converging nozzle [6, 9]. The drawback of this model is that it does not take friction into account. Another possibility in modelling leakage flows is to use the compressible adiabatic flow with friction, known as Fanno Flow, as presented in [11]. In [10], Bell et al. presented an empirical frictional correction factor for the isentropic nozzle model which is derived by calculating the mass flow through variable area leakage paths with real gas properties and then it is correlated to the prediction of an isentropic nozzle model. But this model can be used only when the flow is not choked. From the analysis of 3D CFD calculations it could be seen that in the leakage paths inside the twin screw expander and for the working conditions presented in this paper, flow is usually chocked. Therefore, authors used the isentropic converging nozzle model in this paper.

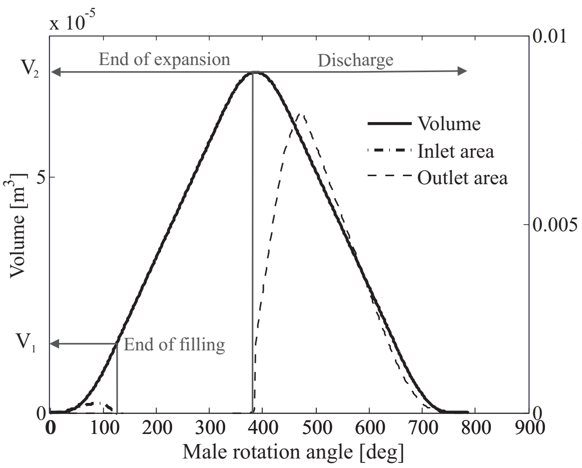
The aim of this paper is to present a mathematical model of a twin screw expander and to validate it with Computational Fluid Dynamic (CFD) results. Moreover, the goal is to extract the coefficients used in the isentropic converging nozzle leakage model from the 3D CFD analysis. The CFD analysis of the twin screw expander has been presented by the authors in [8, 12]. However, additional calculations and analysis were done in these CFD simulations in order to get enough data for accurate model comparison. In the end, performance prediction from the proposed mathematical model is validated with CFD results.

2. Twin Screw Analysis

The geometry of the twin screw expander analysed in this paper is shown in figure 1a. It is a standard air compressor used in opposite sense of rotation together with R245fa instead of air. The configuration of the rotor lobes is 4/6 (male/female). The outer diameter of the male and female rotors is approximately $70mm$ with the L/D ratio of 1.9.



(a) Geometry



(b) Volume of the chamber

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

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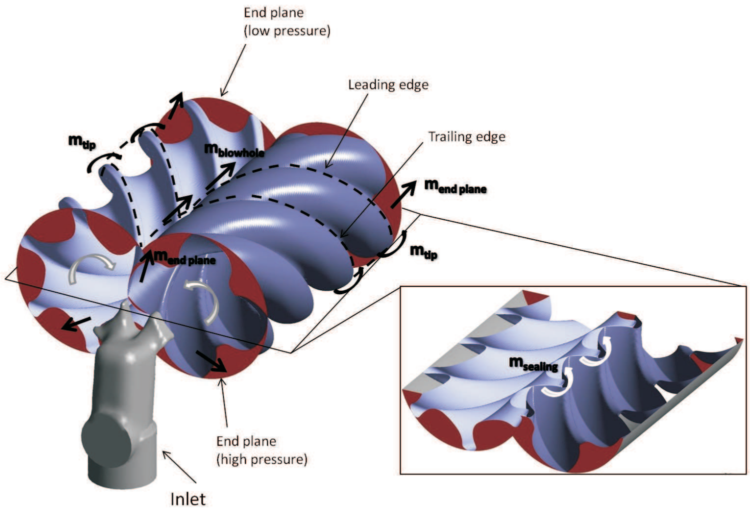


Figure 2: Different leakage types inside the twin screw expander

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 rotors rotate, the volume of the chamber is rising together with the increase in the 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 as shown in figure 2. All leakages are characterized by the length of the leakage path and the area of the clearance.

3. Mathematical model of a twin screw expander

Since the fluid enters through the boundaries of the working chamber, the zero dimensional mathematical model described in this paper represents an open thermodynamic system. The mathematical model 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.

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

- 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
- The heat transfer between 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
- Working fluid of the screw expander is R245fa which is described by Aungier Redlich-Kwong Equation of State (ARK EoS)
- Leakage flows through the end planes are not included in the model since they are not modelled in the CFD calculations

- Once the chamber is connected to the outlet port, the pressure in the working chamber is equal to discharge pressure.

The conservation of mass for the chamber which represents the control volume can be expressed as follows:

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

Energy conservation law applied to the control volume is defined as:

$$\frac{dE}{dt} = -p\frac{dV}{dt} + \sum_i \dot{m}h_i + \dot{Q} \tag{2}$$

If the process is assumed to be adiabatic with conservation laws converted into derivatives of temperature with respect to time, the rate of temperature changes is as follows:

$$\frac{dT}{dt} = \frac{-T\left(\frac{\partial\rho}{\partial T}\right)_v \left[\frac{dV}{dt} - v\frac{dm_{ch}}{dt}\right] - h\frac{dm_{ch}}{dt} + \sum_i \dot{m}_i h}{m_{ch}c_v} \tag{3}$$

The properties of the working fluid are calculated by using the same EoS as used in CFD calculations [8, 13]. The 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 [14]:

$$\dot{m}_{nozzle} = CA\sqrt{p_{up}\rho_{up}}\sqrt{\frac{2k}{k-1}\left(p_{ratio}^{2/k} - p_{ratio}^{(k+1)/k}\right)} \tag{4}$$

Where the function of pressure ratio is defined as:

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

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:

$$W_{ind,cycle} = \int_{cycle} V dp \tag{5}$$

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

$$P_{ind} = \frac{W_{ind,cycle}zn}{60} \tag{6}$$

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

4. 3D CFD analysis of twin screw expander

In this paper, 3D CFD (Computational Fluid Dynamics) calculations of a twin screw expander are used for a validation of the developed mathematical model.The flow calculations inside a screw expander are performed using Ansys Fluent with the use of User Defined Functions (UDFs) to handle the grid movement and real gas model as presented in [8]. 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.

To obtain good comparison between models following constraints are satisfied:

- The same EoS is used in both the 3D CFD calculations and the proposed mathematical model
- To obtain the flow coefficient for different leakage types, results of CFD calculations were used for every angular position. The mass flow rates through the corresponding leakage path were correlated with the pressure ratio between chambers that are forming that leakage path and it's area
- Pulsations in the pipe before the inlet port are obtained from the results of CFD calculations and are used in the developed mathematical model

By analysing the results of CFD calculations, it was seen that pulsations in the pipe before the inlet port 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. Since the aim of this study was to develop the mathematical model of the working chamber of the screw expander, the conditions of the inlet port were obtained from the results of CFD calculations as shown in figure 3. The results of pressure pulsations were calculated through the reference plane as shown in figure 3.

5. Results

The results of the CFD analysis and the developed model have been compared for a few parameters. The first parameter is the performance of the twin screw expander. This is evaluated through the P-V indicator diagram for both models shown in figure 4a. It can be seen that the developed model predicts the pressure in the working chamber well. Using the P-V diagram, power has been calculated using eq. 5 and eq. 6. The difference in power prediction is around 2%.

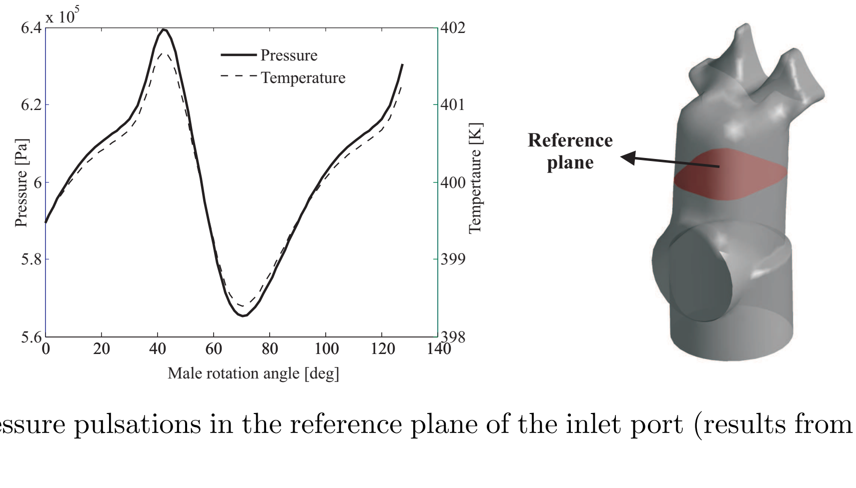
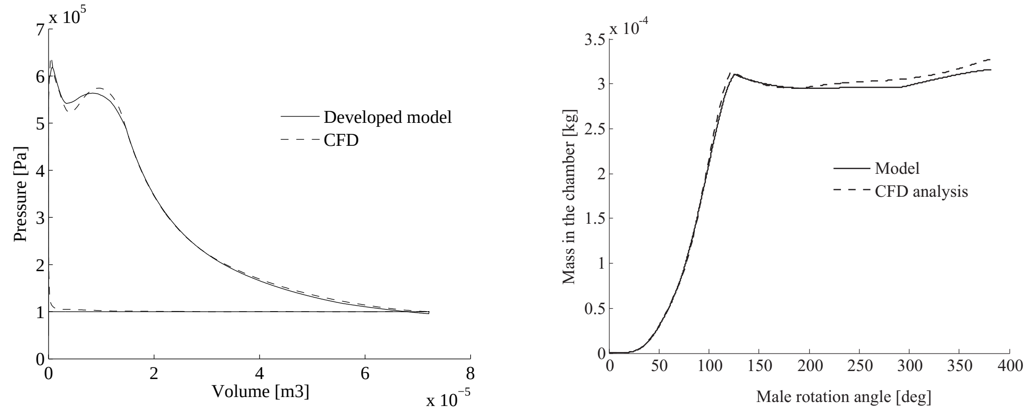


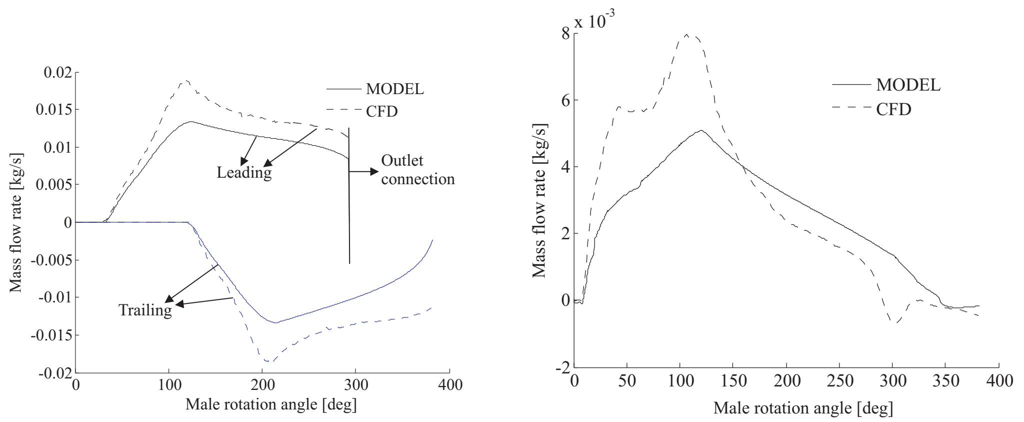
Figure 3: Pressure pulsations in the reference plane of the inlet port (results from CFD analysis)

The second parameter is the mass in the working chamber. The comparison between the models is shown in figure 4b. This parameter is very important because it shows if the mass in the chamber after the filling is approximately the same compared to the CFD results. But also, it shows if the leakage flows are reducing the mass in the chamber in the same way as in CFD results.



(a) P-V indicator diagram (b) Mass in the working chamber

Figure 4: Model predicted and CFD calculated results in the screw expander with pressure ratio 6 and rotational speed of 6000rpm



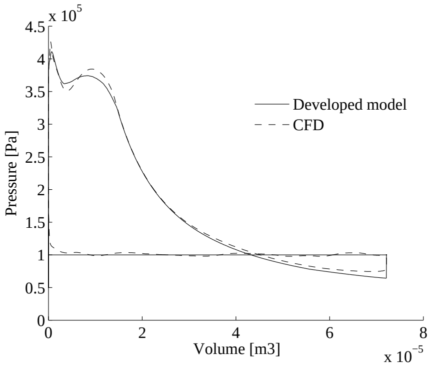
(a) Tip Leakages (b) Sealing leakage

Figure 5: Model predicted and CFD calculated results in the screw expander with pressure ratio 6 and rotational speed of 6000rpm

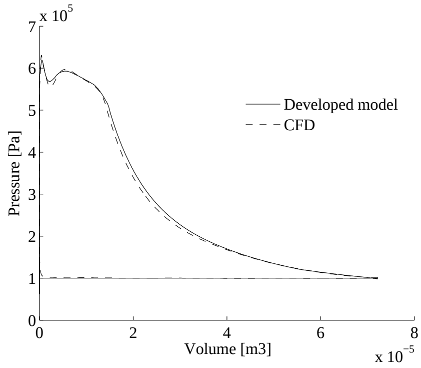
The last two parameters are the mass flow rates through the tip and sealing leakage path. Here it is very important to see if using the constant flow coefficient derived from the CFD calculations can estimate these flows correctly. It can be clearly seen that the trend of these curves is matching well with CFD results. It is important to note that the flow rates are small compared to the flow rate through the machine.

5.1. *Evaluation of the model for different pressure ratio and rotational speed*

Additionally, comparison has been made with a different pressure ratio and rotational speed as shown in figure 6a and figure 6b. The difference in power and mass flow rates between the CFD



(a) Pressure ratio 4 and 6000 rpm



(b) Pressure ratio 6 and 4000rpm

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
4	6000	0.0955	2.18	0.0922	2.05
6	4000	0.1055	3.18	0.1028	3.23

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

and the developed model are presented in Table 1. The biggest difference is for the rotational speed of 4000rpm which is to be expected since the influence of the leakages is higher at lower speeds. It is important to note that coefficients of the model have not been adjusted for these changes in pressure ratio and speed.

6. Conclusion

A mathematical model for calculating the performance of a twin screw expander has been developed. As the input for the developed mathematical model, geometrical parameters such as volume, inlet and leakage areas are provided to the model. Additionally, the pressure and the temperature in the inlet port as a function of rotational angle should be provided to the model. These data can be obtained from the CFD calculations or a 1D model. The model shows good agreement compared to the CFD results. Further improvement will be done in the inlet model which in this moment shows the biggest difference compared to the CFD results.

7. Acknowledgement

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Nomenclature

Symbols

$\dot{m}$ Mass flow rate (kg/s)
$\dot{Q}$ Heat transfer rate (kW)
ρ Density (kg/m^3)
A Area of the leakage path/inlet area (m^2)
C Flow coefficient $(-)$
E Energy (kJ/kg)
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

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

Acronyms

CFD	Computational Fluid Dynamics
EoS	Equation of State
ORC	Organic Rankine Cycle
RKA	Redlich-Kwong Aungier

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