

# **PRELIMINARY MODELLING OF TWO-PHASE EXPANSION USING A COMMERCIAL SINGLE-PHASE SCROLL EXPANDER**

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# **ABSTRACT**

Two-phase expansion is an emerging technology, where R&D activities are accelerating but remain largely in the theoretical domain. REGEN-By-2 project aims to bridge the gap and bring two-expansion in a close-to market level, by developing and experimentally validating prototype two-phase expanders, integrated in a novel patented thermodynamic cycle. The first step of this goal includes the theoretical modelling of two-phase scroll expanders. Within this context, a deterministic two-phase expander model has been developed based on the adaptation of a single-phase scroll compressor model to simulate in detail the performance of a commercial single-phase scroll compressor in two-phase expansion regimes. This study presents an overview of the deterministic model that was developed as well as simulation results that have been derived by means of sensitivity analysis for different operating conditions for a particular commercial scroll geometry. According to the simulation results, it was determined that the relationship between key operating parameters (isentropic/volumetric efficiency and mechanical power) of the expander with the pressure ratio and the rotational speed of the machine follows the findings of in experimental studies on single-phase expanders. This showcases that, in principle, the proposed deterministic model methodology could be used as a tool for the prediction of the behavior of such machines. Nevertheless, a significant shortcoming of the approach is the calculation of extremely low volumetric efficiencies. This suggests that further work is needed in the development of accurate flow models for the prediction of the mass flow rate of two-phase flows, accompanied by more efforts to develop accurate leakage models that are based on two-phase flows.

# **1 INTRODUCTION**

The continuous increase in the global energy demand along with the environmental concerns over the use of fossil-based power systems has been a pivotal motivation towards the faster transition to more sustainable energy solutions (Al-Shetwi, 2022). Organic Rankine cycles (ORC) can offer a promising solution in medium and low temperature heat sources, including waste heat recovery streams, solar thermal systems and biomass (Karellas & Braimakis, 2016). Over the past decade, several studies have been conducted in the fields of ORC technologies, with particular focus in system and specific components design optimization (Carraro et al., 2017; Roumpedakis et al., 2021). A number of researchers have delved into the feasibility of novel thermal cycles, as modifications to the conventional ORC, including the thermodynamic cycles in which the expansion takes place in two-phase region (Braimakis & Karellas, 2023; White, 2021).

Towards the feasibility assessment of thermodynamic cycles implementing a two-phase expansion process, it is necessary to develop and validate a detailed modelling approach for the simulation of the two-phase expanders. Given the fact that two-phase expansion mechanisms in scroll expanders have not yet been thoroughly analyzed, semi-empirical models are not considered as an ideal choice for the

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needs of simulation, in particular due to the imposed limitations in data extrapolation of their predictions (Dumont, Dickes, & Lemort, 2017).

On the contrary, deterministic models are based on control volumes analyses and thus require detailed data for the expander's geometry for an accurate prediction of its performance (Quoilin, Lemort, & Lebrun, 2010). In particular, the deterministic models are using the detailed geometrical characteristics of the expander to associate the defined geometry and the thermodynamics of the expansion process (Cuevas, Lebrun, Lemort, & Winandy, 2010).

Initially, the deterministic models were developed for the simulations of scroll compressors. Nieter (1988) and Nieter and Gagne (1992) set the structure for the development of the first deterministic models by establishing a detailed modelling approach for the suction and the discharge in scroll compressors. One of the first studies to develop a deterministic model for a variable speed scroll compressor with refrigerant injection was published by Park, Kim, and Cho (2002). The results of the simulations were compared against experimental data, revealing a deviation of less than 10% compared to the measurements. Wang, Li, and Shi (2005) proposed a general geometrical model for a scroll compressor, by using discretional involute initial angles to calculate the scroll wraps, working chamber volume and leakage areas. Leclercq and Lemort (2022) developed a dedicated deterministic mode to investigate the operation of a two-phase scroll compressor, calculating isentropic efficiencies below 70% for higher pressure ratios, while additional under-compression losses were reported in two-phase compression.

On the contrary, there is limited literature on deterministic models for scroll expanders. Yanagisawa, Fukuta, Ogi, and Hikichi (2001) developed a scroll expander model on the basis of adapting a scroll compressor model. The main conclusion of the analysis was that the mechanical losses induced by the orbiting motion of the moving scroll had the highest contribution to the expander's efficiency drop. Dickes (2013) developed a deterministic model to analyze the expansion mechanisms of a variable wall thickness two-stage scroll expander. The investigated model was a modification of a developed model from Dechesne (2012) by accounting also for the mechanical losses within the thermodynamic analysis of the previous model. Mendoza, Lemofouet, and Schiffmann (2017) developed a deterministic model to analyze the losses mechanisms of a co-rotating scroll expander both dry and with water injection. The validation of the simulation results against experimental data revealed an error of  $\pm 12\%$ , corresponding to an uncertainty in the exhaust temperature of  $\pm 4$  K.

Although deterministic models have been developed and validated, as was described above, there is yet not, to the best of the authors' knowledge, a relevant study analyzing a scroll expander performing a two-phase expansion and the corresponding modifications that need to be applied in the respective modelling approach. This study presents the preliminary modelling for the two-phase expansion of a scroll expander, by retrofitting a developed deterministic model for single phase expanders. The simulation results are assessed based on analytical geometrical data from a commercial single phase scroll expander and the influence of key model parameters was verified based on dedicated sensitivity analyses.

# **2 METHODOLOGY**

### **2.1 General description of the deterministic expander model**

The two-phase deterministic expander model presented in this work is based on the single-phase scroll compressor model developed by Bell (I. Bell, 2011). An open-source version of the model built in Python programming language is freely available, integrated into the PDSim software package (Ian H. Bell et al., 2020), using open-source Coolprop software (Ian H Bell, Wronski, Quoilin, & Lemort, 2014) for the calculation of refrigerant properties. The presented expander model has been developed in Matlab (Matlab, 2012) carried out by implementing a series of modifications to enable the simulation of two-phase expansion. It is noted that regardless of the different interface, the present model shares the same principles and employs the same simulation and solution approaches. An outline of the deterministic expander model is shown in Figure 1.

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**Figure 1:** Outline of deterministic expander model

The core of the model includes a set of control volumes (CVs), which correspond to the pockets (chambers) created by the fixed and orbiting scroll during the revolution of the machine. During the rotation of the machine, the volumes of the CVs change causing the fluid which they contain to compress or expand (depending on the revolution angle and scroll geometry). At the same time, CVs may exchange mass with neighboring CVs, if there is an available open flow path, through other CVs if there are available leakage openings, or, in the case of CVs corresponding to suction and discharge chambers, the inlet and outlet tubes. Meanwhile, heat is exchanged between the working fluid and the scrolls as it flows through the inlet and outlet tubes and during its expansion/compression inside the CVs, as well as between the scrolls and the ambient. Considering the above, the main components of the model are the following:

- 1) Mass and energy balance inside each CV
- 2) Flow models to calculate the mass flow rate of the working fluid along primary and leakage flow paths
- 3) Pressure drop models to calculate the pressure drop of the working fluid in the inlet/outlet tubes
- 4) Heat transfer models to calculate the heat exchanged in the inlet/outlet tubes and inside each CV
- 5) Overall energy balance model of the scrolls

The main inputs and outputs of the model are summarized in **Table 1**.





The inputs to the expander model include the scroll machine geometry, the working fluid inlet state, the outlet pressure, the rotational speed and the ambient temperature. The scroll geometry is determined based on a set of independent geometrical parameters of the machine, which are summarized and explained in **Table 2** (commercial scroll compressor model). Based on these fundamental parameters, it is possible to calculate the volumes of the CVs, as well as the primary and leakage flow areas between different CVs as a function of the revolution angle  $(\theta)$ .

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A visualization of the definitions of the main scroll geometric parameters is included in **Figure 2**.



**Figure 2:** Visualization of the definitions of main scroll geometry parameters (I. H. Bell, 2011)

In the following sections, the components of the deterministic model are described.

#### **2.2 Control volume energy and mass balance**

In the developed model, homogeneous two-phase flow (uniform fluid properties) and negligible change of kinetic and gravitational potential energy have been considered. Furthermore, because of substantial uncertainty of the heat transfer conditions inside the scroll chambers and the lack of validated heat transfer correlations, no heat transfer is assumed to take place inside the CVs.

The mass balance equation in each CV at a given timestep is described by the following equation:

$$
\frac{dm_{CV}}{dt} = \sum_{f}^{P} \dot{m} \tag{1}
$$

In the above equation,  $m_{CV}$  is the mass contained in a CV while  $\sum_f^p m$  is the net mass flow rate of the working fluid entering/leaving the CV through p flow paths which exist at the given timestep. Moreover, the energy balance equation for each CV is the following:

$$
\frac{du_{CV}}{dt} = \frac{dQ}{dt} + p\frac{dV}{dt} + \sum_{1}^{p} \dot{m}h
$$
 (2)

The energy balance takes into account the heat exchanged between the working fluid and the scroll wraps  $\left(\frac{dQ}{dt}\right)$ , the boundary work  $\left(p\frac{dV}{dt}\right)$  produced during the change of the CV volume, as well as the energy entering/leaving the CV due to inward and outward mass flow of working fluid  $(\sum_1^p m h)$  through p flow paths which exist at the given timestep.

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Additionally,  $u_{CV}$  and  $p$  are the (uniform) internal energy and pressure of the working fluid inside the  $CV$ , while  $V$  is its volume.

The integration of the above two equations enables the calculation of the thermodynamic state of each CV at the next timestep/rotation angle  $(t+1)$  based on the values of the current timestep/rotation angle (t).

## **2.3 Flow models**

During the rotation of the scroll machine, a series of primary and leakage flow paths are formed, causing the working fluid to flow from one CV to another or between inlet/outlet CVs and respective tubes. Primary flow paths refer to the flow paths between CVs and tubes which are openly interconnected and include large flow areas. Leakage paths, on the other hand, appear between non-openly interconnected CVs due to small orifices. In both cases, appropriate flow models are used for calculating the mass flow rate of the primary flow and the leakage paths in the scroll machine based on their flow area and pressure difference. For details on the calculation of primary and leakage flow areas, the reader is prompted to the work carried out by Bell (I. H. Bell, 2011) and Peng et al. (Peng, Zhu, & Lemort, 2016).

The flow along primary flow paths is similar to the flow in a convergent nozzle and is thus considered adiabatic and compressible. For two-phase adiabatic compressible flow in a nozzle, the Chisholm model (Chisholm, 1985) is used for calculating the mass flow rate ( $\dot{m}$ ) based on the upstream ( $p_{\mu\nu}$ ) and downstream pressure ( $p_{down}$ ) and effective specific volume ( $v_e$ ) of the fluid (I. Bell, 2011; Chisholm, 1985) and slip ratio  $K$ :

$$
\dot{m} = X_d C_d A_{th} \sqrt{\frac{2 \int_{p_{down}}^{p_{up}} v_e dp}{v_{e,down}^2 - \sigma v_{e,up}^2}}
$$
\n(3)

$$
u_e = \left[x \cdot u_g + K_e \cdot (1 - x)u_l\right] \left[x + \frac{(1 - x)}{K_e}\right] \tag{4}
$$

$$
K_e = \psi + \frac{(1 - \psi)^2}{K - \psi} \tag{5}
$$

$$
K = \psi + (1 - \psi) \left\{ \frac{1 + \psi \cdot \frac{(1 - x) \cdot u_l}{x \cdot u_g}}{1 + \psi \cdot \frac{(1 - x)}{x}} \cdot \sqrt{\frac{u_g}{u_l}} \right\}
$$
(6)

The integral of Equation (3) is calculated numerically, considering isentropic expansion from the upstream to the downstream pressure. In principle,  $v_e$  depends on the extent of homogeneity of the twophase flow as expressed by  $\psi$ . More specifically, for  $\psi = 0$  and  $\psi = 1$  the fluid is treated as liquid and completely homogeneous, respectively. Following the proposal by Chisholm (Chisholm, 1985), it is calculated for  $\psi = 0.4$ . Furthermore,  $X_d$  is the area correction factor  $(X_d = 1)$ ,  $C_d$  is the discharge coefficient ( $C_d = 0.77$ ),  $A_{th}$  is the throat area of the flow path (calculated for each revolution angle based on the scroll geometry) and  $\sigma$  is the area ratio of downstream to upstream flow areas which is difficult to calculate analytically. In the present work, it can be assumed that  $\sigma = 0$ , a value which yields the lowest possible mass flow rate (I. H. Bell, 2011).

Regarding primary flows, the set of equations are used directly for mass flow rate calculation. Regarding leakage flows, the Chisholm model is also used, however the calculated mass flow rate is multiplied by a correction factor  $(M)$  that has been derived based on regression using experimental data for singlephase compression of working fluids  $N_2$ ,  $CO_2$ , R134a and R140a (I. H. Bell, 2011):

$$
\dot{m}_{corr,leak} = \frac{\dot{m}}{M} \tag{7}
$$

#### **2.4 Heat transfer and pressure drop models**

Heat transfer models are used for calculating the heat exchanged between the working fluid and the scroll machine as it flows through the inlet/outlet tubes and inside the scroll wraps. In the present work, heat transfer has been modelled only for the inlet/outlet tubes. The heat exchanged is calculated according to the following formula:

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$$
\dot{Q}_{tube} = \alpha \cdot (T_{scroll} - T_f) \cdot D \cdot \pi \cdot L \tag{8}
$$

Parameters D and L represent tube diameter and length, respectively, while  $T_{scroll}$  and  $T_f$  express the temperature of the tube wall (which is considered identical to the temperature of the whole scroll machine, as it was stated previously) and working fluid, respectively. The heat transfer coefficient  $\alpha$  is calculated depending on the state of the working fluid flow (single-phase, evaporation or condensation). For single-phase heat transfer, the Gnielinski correlation designs (Bergman, 2011) is used, while the Shah correlations are used for evaporation (Mirza M. Shah, 1982) and condensation (M. M. Shah, 1979). For pressure drop calculation, the Churchill (Churchill, 1977) and Blasius (Blasius, 1913) correlations are used for single- and two-phase flow, respectively.

#### **2.5 Scrolls energy balance**

A lump energy balance approach is used for implementing the energy balance on the scrolls, which is considered to be at uniform temperature  $(T_{scroll})$ . Heat is exchanged between the scroll shell and the ambient  $(\dot{Q}_{amb})$ , according to the following equation:

$$
\dot{Q}_{amb} = h_{amb} \cdot A_{shell} \cdot (T_{scroll} - T_{amb}) \tag{9}
$$

In the above equation,  $h_{amb}$  is the free convection heat transfer coefficient between the scroll shell and the ambient  $(h_{amb} = 0.02 \text{ kW/m}^2\text{K}$  (Bergman, 2011)), while  $A_{shell}$  is the total external surface of the shell, determined by its geometry.

Meanwhile, it is assumed that the mechanical losses of the scroll  $(W_{mech, loss})$  are converted into heat which is absorbed by the shell. A simplified approach is followed for the calculation of the mechanical losses, by considering a fixed mechanical efficiency of the scroll  $(\eta_{mech})$ , according to the equation:

$$
\dot{W}_{mech,loss} = (1 - \eta_{mech}) \cdot \dot{W}_{PV} = \dot{m}(1 - \eta_{mech})(h_{in} - h_{out})
$$
\n(10)

At steady state conditions, the sum of the net thermal energy absorbed by the scrolls by the working fluid in the tubes and the mechanical losses is equal to the thermal energy rejected by the scroll to the ambient:

$$
\dot{Q}_{tubes} + \dot{W}_{mech,loss} = \dot{Q}_{amb}
$$
\n(11)

#### **2.6 Model solver**

The solver of the model is described in the flow diagram of **Figure 3**.



**Figure 3:** Deterministic model solution algorithm

The solver is based on two nested error checking loops. The outer loop is based on discharge enthalpy convergence while the inner loop is based on convergence of the scroll temperature and the working fluid states in the CVs for  $\theta = 0$  and  $\theta = 2\pi$ , since steady state operation is assumed. Initially, a discharge enthalpy is guessed. For this discharge enthalpy, the equations presented in the previous sections are integrated for a whole revolution (from  $\theta = 0$  to  $2\pi$ ). This allows the calculation of the state of the working fluid in the CVs at the end of the revolution as well as the net heat transfer in the scrolls. Based on these values, two error terms are calculated corresponding to the deviation of the working fluid in the CVs at the start/end of revolution ( $error_{CV,tot}$ ) and a residual related to scrolls heat balance (error<sub>scrolls</sub>):

$$
error_{CV,tot} = \sqrt{\sum_{i}^{n} error_{CV,i}}
$$
 (12)

$$
error_{CV,i} = \left[ \frac{|T_{i,\theta=2\pi} - T_{i,\theta=0}|}{T_{i,\theta=0}} \right]^2 + \left[ \frac{|\rho_{i,\theta=2\pi} - \rho_{i,\theta=0}|}{\rho_{i,\theta=0}} \right]^2 \tag{13}
$$

$$
error_{scrolls} = \dot{Q}_{tubes} + \dot{W}_{mech,loss} - \dot{Q}_{amb}
$$
\n(14)

If both of these error terms are higher than a tolerance thershold, the calculated values of the working fluid state at  $\theta = 2\pi$  are used as initialization values for the next revolution, while a new scroll temperature is assumed. The process is repeated for consecutive revolutions until both error terms are reduced below the threshold.

In the next step, the calculated discharge enthalpy is calculated, defined as the mass-weighted average enthalpy of the working fluid at the inlet of the outlet tube of the machine:

$$
h_{disc} = \frac{\sum_{0}^{2\pi} \dot{m}h}{\sum_{0}^{2\pi} \dot{m}}
$$
 (15)

The discharge enthalpy is compared with the guessed discharge enthalpy. If the difference is higher than a threshold, a new discharge enthalpy is assumed and the whole process is repeated. Iterations with new guess values of the discharge enthalpy are repeated until convergence is achieved.

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### **2.7 Definition of control volumes**

An important aspect of the modelling approach is related to defining, numerical handling of splitting, merging and inheritance of properties of CVs based on their creation, succession and disappearance of scroll chambers. For brevity, the above issues are not elaborated in the present study. For a detailed description, the reader is prompted to the work by Bell (I. H. Bell, 2011).

### **2.8 Expander performance evaluation indexes**

Two main expander performance evaluation indexes are the overall isentropic and volumetric efficiency of the expander, which are defined according to the following equations:

$$
\eta_{is} = \frac{W_{net}}{\dot{m}_{wf}(h_{in} - h_{disc,is})} = \frac{\eta_{mech}W_{PV}}{\dot{m}_{wf}(h_{in} - h_{disc,is})} = \eta_{mech}\frac{\sum \int_{0}^{2\pi} p dV}{\dot{m}_{wf}(h_{in} - h_{disc,is})}
$$
(16)

$$
\eta_{vol} = \frac{\dot{m}_{wf}}{\omega/2\pi \cdot V_{disp}/V_{ratio} \cdot \rho_{in}} \tag{17}
$$

It is noted that in the present work, the volumetric efficiency is defined as the ratio of the actual to the theoretical mass flow rate of working fluid displaced by the expander. In several studies, the volumetric efficiency is defined as the reverse of this ratio (called filling factor).

## **3 RESULTS**

Simulation results are presented for the set of conditions shown in Table 3. A parametric investigation is carried out for the conditions which are summarized in **Table 3**.





In all simulations, the ambient temperature is kept constant, equal to 25℃, as well as the outlet saturation temperature, which is considered equal to 30℃, corresponding to a saturation pressure of 1.54 bar. Three different vapor quality values at the inlet of the expander are investigated, equal to 0.70, 0.75 and 0.75. Furthermore, the expander inlet pressure is determined by considering a variation of the inlet saturation temperature from 60℃ to 90℃ in increments of 5 K. It is noted that the pressures corresponding to these range of saturation temperature range from 3.91 bar to 8.33 bar, thus for an outlet expander pressure of 1.54 bar, the pressure ratio varies from 2.52 to 5.39. The simulations are carried out for two rotational speeds corresponding to 3000 and 5000 RPM.

The results of the parametric analysis are summarized in **Figure 4**. For each set of input variables, the isentropic and volumetric efficiency of the expander are calculated, along with the working fluid mass flow rate and mechanical power.



**Figure 4:** Deterministic model simulation results

From a qualitative perspective, the variation of all investigated parameters (isentropic efficiency, volumetric efficiency and mechanical power) is similar to that of single-phase scroll expanders, as reported in experimental literature studies (Declaye, Quoilin, Guillaume, & Lemort, 2013; Lemort, Quoilin, Cuevas, & Lebrun, 2009; Mendoza, Navarro-Esbrí, Bruno, Lemort, & Coronas, 2014). This similarity showcases the general applicability of the deterministic model for the simulation of scroll expanders.

Regarding the isentropic efficiency, it can be observed that is shows a considerable variation for different operating conditions, ranging from a minimum of about 68% to a maximum of 85%. Overall, higher isentropic efficiencies are achieved for lower rotational speeds. It can be observed that for the higher rotational speed (5000 RPM), there is an optimal pressure ratio between 3 and 3.5 which maximizes the isentropic efficiency of the expander, which is about 80%. On the other hand, if the rotational speed is reduced to 3000 RPM, there is a negative correlation between the pressure ratio and the isentropic efficiency. Therefore, the highest isentropic efficiency (85%) is attained for the lowest pressure ratio around 2.5. Meanwhile, there is a positive correlation between the quality at the expander inlet and the isentropic efficiency, which is more intense for higher rotational speed.

The calculated mass flow rate of the working fluid going through the expander shows a linear relationship with the pressure ratio. As expected, significantly higher mass flow rates are achieved for the higher rotational speed (5000 RPM). Meanwhile, there is a decline in the mass flow rate for decreasing vapor qualities. This effect can be explained based on the increasing density of the working fluid for decreasing vapor qualities because of the increasing liquid phase fraction.

Although the mass flow rate shows a linear correlation with the pressure ratio, the volumetric efficiency is almost independent of it. Interestingly, the volumetric efficiency seems to be dependent only on the quality at the expander inlet (higher qualities resulting in higher volumetric efficiencies) and the rotational speeds (higher rotational speeds resulting in lower volumetric efficiencies). Overall, the volumetric efficiency ranges between around 67% to a maximum of 81%. Considering the definition of the volumetric efficiency that is used for the calculations in the present work and considering the effect of leakages, the volumetric efficiency would be expected to be significantly higher (>1). These results indicate the probable inadequacy of the employed leakage or possibly more broadly the flow model based on Chisholm methodology to accurately predict the mass flow rate of two-phase flows for the particular working fluid and operating conditions. Some possible reasons for this are the following:

• Uncertainty in value of nozzle area ratio  $(\sigma)$  parameter. Higher values result in higher mass flow rates, however increasing the value of the parameter to higher values results in numerical errors because of negative values being calculated in the root term of Equation 3.

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- Uncertainty in the homogeneity state of the flow. As it was described previously, for the present calculation a moderately homogeneous flow has been considered for mass flow rate calculations, using a  $\psi$  parameter equal to 0.44 for the calculation of the slip ratio.
- Uncertainty in the regression coefficients used for the calculation of the correction factor used in leakage flow calculation  $(M)$ . As it was mentioned, this correction factor is derived based on experimental data for single-phase compression of different working fluids other than R1233zd(E) and is possibly unsuitable for the conditions presented in the present work.

Regarding the mechanical power produced by the expander, it shows a linear correlation with the pressure ratio. Meanwhile, much higher power outputs are observed for higher rotational speeds. The effect of the vapor quality at the expander inlet on the power output is very minor.

## **4 CONCLUSIONS**

In the present work, the simulation results of a deterministic two-phase scroll expander model that is based on the modification of a single-phase scroll compressor model were presented for different sets of operating conditions. In general, the relationship between key operating parameters (isentropic/volumetric efficiency and mechanical power) of the expander with the pressure ratio and the rotational speed of the machine is similar to that reported in experimental studies on single-phase expanders. This showcases that, in principle, the deterministic model methodology that has been developed in the present study could be used as a tool for the prediction of the behavior of scroll expanders. Nevertheless, a significant shortcoming of the modelling approach is revealed by taking into account the extremely low values of calculated volumetric efficiency, which is in all cases far lower than unity despite anticipating values higher than 1 according to its definition in the present work. This suggests that further work is needed in the development of accurate flow models for the prediction of the mass flow rate of two-phase flows. Furthermore, more efforts are needed to develop more accurate leakage models that are based on two-phase flows. Overall, despite its promising capabilities, the deterministic expander model features several empirical factors that should be determined by using experimental data on two-phase scroll expanders, which are currently rather limited.

# **NOMENCLATURE**

## **Abbreviations**



## **Variables**



## **Greek symbols**







 $\mathbf{S}$ 

scroll tubes volumetric working fluid

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