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Article

Numerical Modelling and Experimental Validation of Twin-Screw Expander

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Abstract: Positive displacement machines have been identified as appropriate expanders for small scale power generation systems such as ORCs. Screw expanders can operate with good efficiency for working fluids under both dry and two-phase conditions. Detailed understanding of the fluid expansion process is required to optimise the machine design and operation for specific applications, and accurate design tools are therefore essential. Using experimental data for air expansion, both CFD and chamber models have been applied to investigate the influence of port flow and leakage on the expansion process. Both models are shown to predict pressure variation and power output with good accuracy. The validated chamber model is then used to identify optimum volume ratio and rotational speed for the experimental conditions.

Keywords: twin screw; air; expander; performance; optimisation; chamber model; CFD; validation; built-in volume ratio;

1. Introduction

There is currently significant interest in reducing the global greenhouse gas emissions from industrial processes, which alone account for almost 26% (275 Mtoe/yr) of Europe's energy consumption [1]. Studies looking at global thermal energy availability [2] have shown that about 52% of the primary energy consumption is currently being rejected as waste heat. Of this global waste heat potential, 63% exists as low temperature (< 100°C) heat sources. Waste heat energy recovery systems seem to be an attractive proposition that can potentially reduce energy consumption and help to decarbonise industrial processes.

The Organic Rankine Cycle (ORC) provides a means of extracting useful electrical or mechanical power from heat sources at low temperature levels. However, this power is extracted with a much lower thermal efficiencies than conventional high temperature Rankine cycles. Additionally, low temperature ORC systems generally demand a larger heat exchange area per unit power generation, resulting in higher investment costs for the heat transfer equipment, with considerable work input for the feed pump due to the lower latent heat of evaporation of the organic fluids compared to water. Conventional ORC cycles are usually limited to dry vapour admission to turbines, which leads to the complication of having to remove the superheat before condensation begins, with an associated increase in the surface area required for heat transfer.

The thermal efficiency of ORCs can generally be increased by allowing a higher mean temperature of heat addition (in accordance with Carnot's principle) or by reducing the mean temperature of heat rejection. By allowing expansion to take place within the two-phase region, the ORC system can achieve a higher mean temperature of heat addition to increase the cycle efficiency, and avoid the requirement to desuperheat the working fluid before the condenser, thereby reducing the mean temperature of heat rejection [3]. Allowing two-phase conditions at the expander inlet also reduces

the constraints due the heat exchanger minimum temperature different, leading to better temperature matching of the heat source and working fluid. This offers the potential to increase heat recovery from the source fluid, thereby increasing the net power output.

The potential thermodynamic and economic benefits of ORC systems, including the Trilateral Flash Cycle [4] and their optimisation [5] considering expansion of initially saturated liquid are reported in the literature. Several studies have also looked at the working fluid selection [6] for working in sub-critical and trans-critical ORC cycles [7] using screw expanders. There is, however, a lack of experimental validation for expander performance models used in these studies.

Table 1. Geometrical data of the GL51.2-M twin screw expander

	Male rotor	Female rotor
No of lobes	3	5
Wrap angle	200deg	120deg
Head diameter	72mm	67.5mm
Length		101mm
Built-in volume ratio (V_i)		1.47
Displaced volume per male rotor revolution		285cm ³
Rotor profile	mod. asym. SRM-profile	
HP/LP ports arrangements	Axial and Radial/Axial	
Design Clearance (Interlobe × Radial × HP End × LP End)	50-80μm × 80μm × 100μm × 250μm	

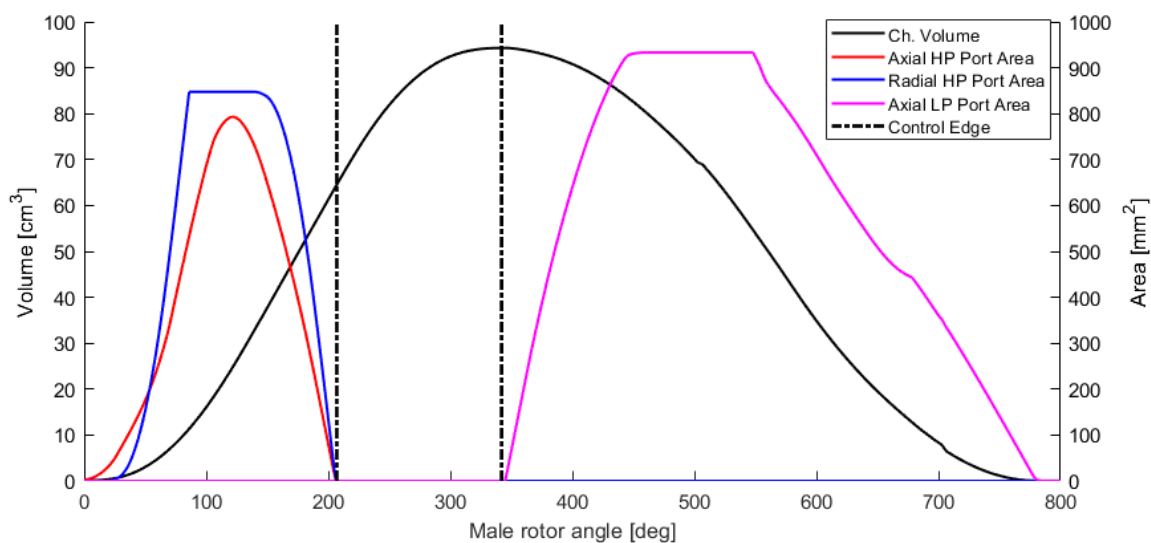


Figure 1. Port areas and volume curve of the screw expander GL51.2-M

The expansion of two-phase, liquid vapour mixtures presents serious challenges for turbomachinery, but can be achieved with good efficiency in positive displacement machines. A number of different types of volumetric expander have been considered for use in small-scale ORC systems, as reviewed by Zywica et al. [8]. The general requirements for high expansion ratio, high isentropic efficiency and low cost mean that scroll, screw, rotary vane and reciprocating piston machines are can be suitable depending on the necessary working fluid, flow rate and system pressure [9]. For power outputs in the tens of kW, screw expanders have been identified as a suitable expander technology for low temperature waste heat recovery applications. In these applications, expansion of the fluid from saturated liquid [10] or two-phase conditions [3] has been shown to allow maximum net power output from a given waste heat source. However, one of the main challenges with two-phase expansion is the large density change, which influences the physical size requirements for positive displacement machines such as screw expanders.

55 High efficiency can be achieved by matching the screw expander's built-in volume ratio, ϵ_v , to
56 the volumetric expansion of the fluid in the process; the maximum value of ϵ_v is however limited due
57 to; geometrical constraints of the screw rotors, increased filling losses due to the decreasing size of the
58 inlet port, and the decreasing mass flow rate for a given machine size. The influence of these different
59 factors makes performance prediction and optimisation of screw expanders essential when considering
60 their use in ORC systems. Thus, it is important to develop a validated model that accurately captures
61 the effect of built-in volume ratio and operating conditions on the expander performance.

62 This paper will focus on the case of single-phase expansion of air using a twin screw expander.
63 The aim is to establish an accurate and reliable model for the expansion of air, while future work will
64 focus on the more complex case of two-phase expansion, leading to a robust tool for general use in
65 performance prediction of power systems. Two modeling approaches will be considered. Firstly a
66 quasi-1D modelling tool based on the 'chamber model' approach [11] has been developed for twin
67 screw expanders. Secondly, 3D CFD modelling has also been performed for comparison. Previous
68 studies by Kovacevic et al. have described the CFD grid generation and calculation methodology in
69 detail [12] and demonstrated good agreement with measured data for screw expander applications
70 [13]. The numerical results were computed for the expander with characteristics defined in (Table 1 and
71 Figure 1) running on single-phase air and compared against the experimental data presented by Hutker
72 et. al. [14]. An extension of this work validating two-phase R245fa expansion is the focus of future
73 research publications. For single or two-phase conditions, the validated model allows evaluation of
74 maximum efficiency maps as a function of built-in volume ratios at different pressure ratios. This will
75 be demonstrated for the air expander considered in this paper. These established performance maps
76 can be used with cycle optimisation tools to evaluate the optimum design of twin-screw expander
77 geometry and its operating conditions for specific applications within power generation systems.

78 2. Modelling

79 Two numerical modelling approaches for twin-screw expanders are presented in this section. The
80 first is a 1D chamber model (1D Ch. Model), which is a computationally efficient approach to solve the
81 system of equations. The second approach considers the expander in its three-dimensional (3D CFD)
82 numerical environment and models the full three-dimensional Navier-Stokes equations with RANS
83 k-e closure for turbulence modelling, which requires several days of computation on high performance
84 clusters. The in-house computational code SCORG© [13] enables use of both chamber modelling and
85 3D CFD in screw machines.

86 2.1. Chamber model (1D Ch. Model)

87 Based on the geometry calculation from SCORG V5.7 (Figure 1), the commercial software
88 GT-SUITE [15] was used to implement the multi chamber modelling approach outlined in the [11].
89 This software models working chamber of the expander and manifolds using chamber modelling,
90 where scalar variables are assumed to be uniform within, while all other flow component are modelled
91 using 1D formulation of the Navier-Stokes equations on a staggered grid spatial discretisation.

92 The expander is divided into various fluid components (Figure 2) such that an inlet pipe
93 connecting a flow-split that feeds the working chambers of the expander, which then allows the
94 fluid to accumulate to another flow split and exit via outlet pipe work. The pipe volumes are divided
95 into sub volumes while the chamber and flow split manifolds are represented by a single volume,
96 while the vector variables are solved at the boundary.

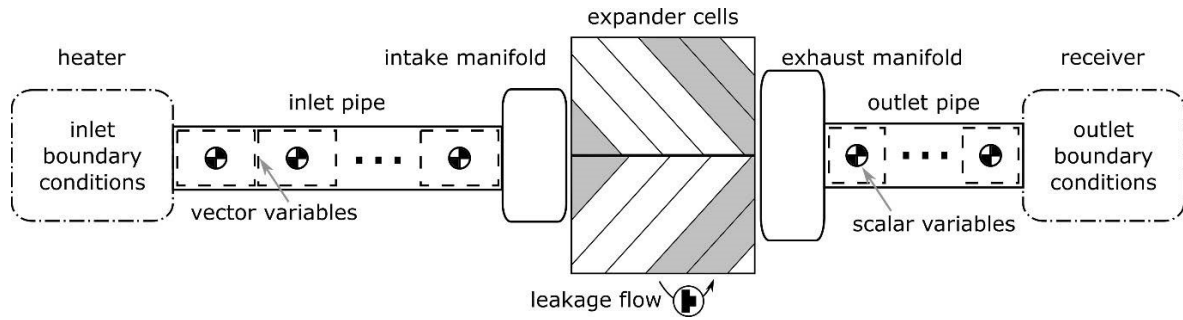


Figure 2. Modelling approach for 1D Ch. Model [10]

97 The chamber volume and the corresponding flow areas for ports and leakage paths are provided
 98 as a function of rotor angle (Figure 1). Currently, no heat transfer is modelled and the walls of the
 99 components are modelled as adiabatic.

100 All fluid components within the 1D Ch. Model including leakage flows are modelled as flow
 101 through an orifice. For the validation case considering gaseous air, the orifice flow is modelled based
 102 on the isentropic nozzle relationships for subsonic and choked flow regimes.

103 For the two-phase environment, the nozzle flow is modeled using incompressible Bernoulli
 104 equation for liquids, and the isentropic nozzle relationships are considered for gases. This requires the
 105 calculation of ratio of specify heat (γ) and dynamic viscosity (μ), which are calculated as an equivalent
 106 property using a weighted average based on the fluid quality (χ) as shown in Eq. (1) and Eq. (2).

$$\gamma_{eqv} = \gamma_{vap}\chi + \gamma_{liq}(1 - \chi) \quad (1)$$

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

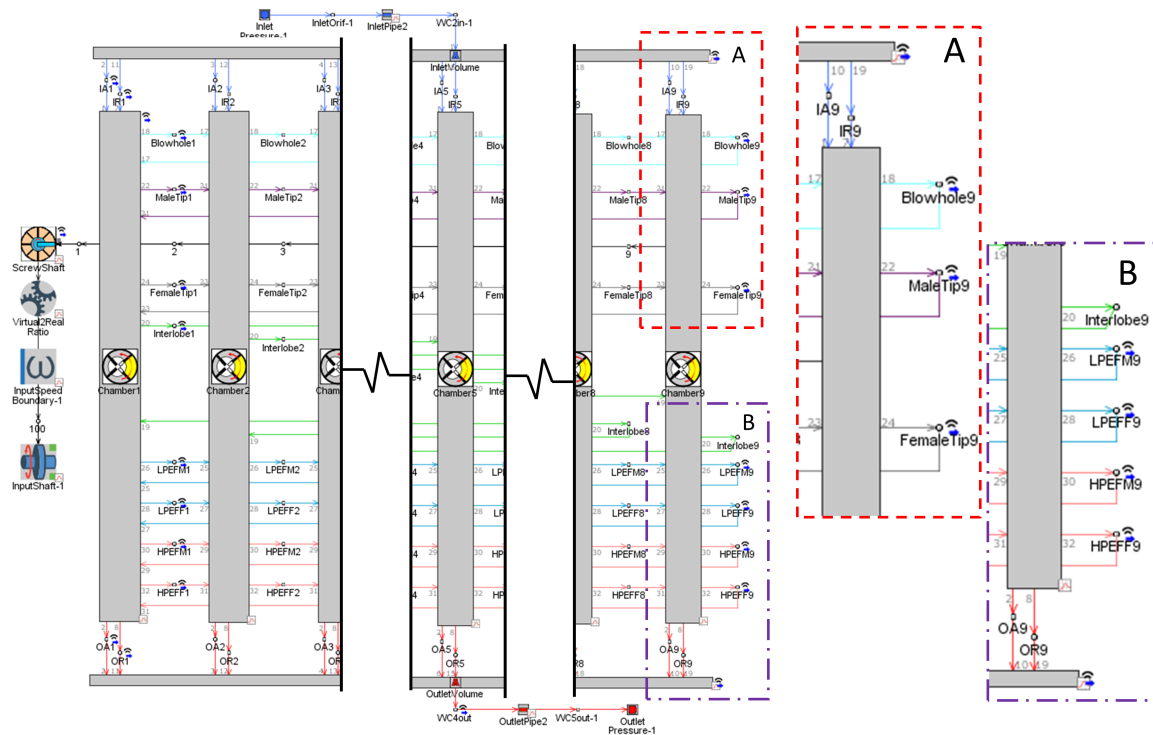


Figure 3. GT-SUITE model of GL51-M Expander, IA = inlet axial port, IR= inlet radial port, OA = outlet axial port, OR = outlet radial port, Male Tip = male rotor tip clearance leakage, Female Tip = female rotor tip clearance leakage, LPEFM = low pressure end face male rotor leakage, LPEFF = low pressure end face female rotor leakage, HPEFM = high pressure end face male rotor leakage, HPEFF = high pressure end face female rotor leakage,

107 The systems of conservation equations are solved using explicit 5th order Runge-Kutta integration
 108 scheme to solve for mass and internal energy. With the known volume and mass, the corresponding
 109 density is calculated. The density and internal energy values are used to then determine the pressure
 110 and temperature via the NIST REFPROP database [16].

111 The GT-SUITE model implementation of the twin-screw GL51.2-M expander is shown in Figure
 112 3. The 3/5 lobed machine is modelled with 9 chambers in total, which is calculated based on the
 113 maximum number of working chambers that the meshing rotors can form at a point in time. All
 114 chambers are connected to the inlet and outlet manifolds and dedicated links are modelled for axial
 115 and radial ports respectively. The leakage paths are also modelled via their own dedicated connections
 116 between the chambers, and it is connected via a cyclic link where the last chamber is connected to the
 117 first chamber in order to allow continuity and leakage access to all possible paths.

118 The explicit solver was set to consider a maximum time step corresponding to 1° solving the
 119 equation for the full cycle (360°). The convergence criteria set at steady-state condition on mass flow
 120 rate and pressure, i.e. 0.2% variation on mass flow rate and pressure in flow connections compared
 121 with the results from the previous cycle.

122 2.2. Computational Fluid Dynamics Model (3D CFD)

123 To assess the quality of the 1D Ch. Model discussed in the previous section, 3D CFD simulations
 124 were conducted and compared against the experimental data. As the working fluid flows through the
 125 machine, the net force exerted by the fluid on the rotors causes rotation, with expansion of the fluid
 126 occurring once the inlet port closes (Figure 4). This results in net power output via the shaft of the
 127 male rotor, which can be used to drive a mechanical load or electrical generator.

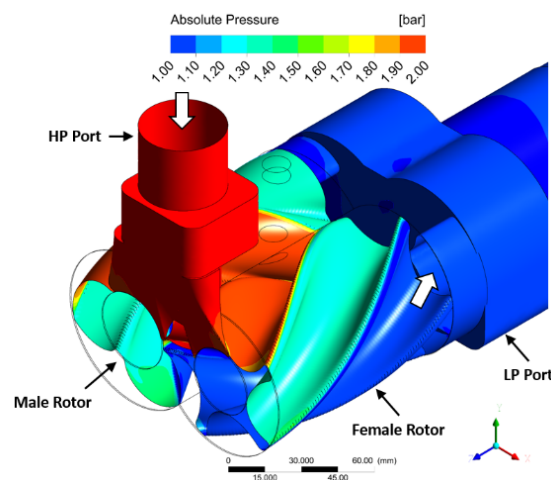


Figure 4. Pressure variation in twin screw expander

128 The computational fluid domain is decomposed into three main regions (Figure 5) namely the
 129 high pressure (HP) port, rotor domain (containing the male and female rotor) and the low pressure
 130 (LP) port. Moreover, the end face clearances were modelled with additional domains attached on
 131 both sides of the rotor; i.e. the HP end face leakage was modelled with additional domain discretising
 132 the space between the HP port and rotor. A numerical (GGI) interface was used to connect all the
 133 computational domains. The rotor domain is updated with a corresponding grid at each time intervals
 134 to model the rotation.

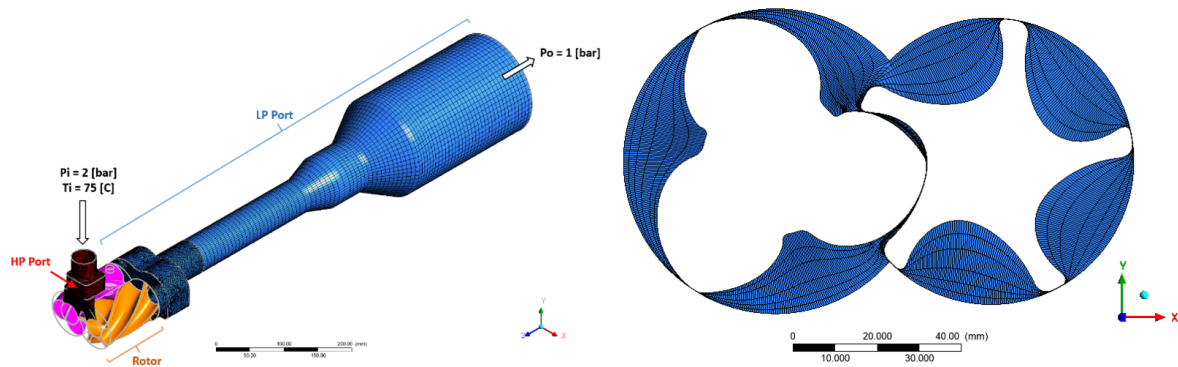


Figure 5. CFD domains with surface mesh for the GL51.2-M twin screw expander

135 The convergence criteria for mass, momentum and energy equations were set to an r.m.s value of
 136 $1E-4$, $1E-3$ and $1E-3$ respectively. Surplus amount of time steps were considered for all simulations
 137 until a cyclic repetition were observed for pressure, power and mass flow rate via the machine.

138 3. Results

139 Numerical simulations were conducted to replicate the experimental conditions reported in [14].
 140 A range of inlet pressures between 1.5-3bar was investigated at an inlet temperature of 75C, with the
 141 expander rotational speed ranging from 1,000-16,000RPM.

142 The design clearance gaps for the GL51-2M expander were defined as $50-80\mu\text{m}$ for the interlobe,
 143 $80\mu\text{m}$ radial and 100 and $250\mu\text{m}$ for the high-pressure (HP) and low-pressure (LP) end faces respectively.
 144 However, due to mechanical and thermal loads these clearance gaps are known to change in operation.
 145 Operational clearance settings of $10\times 80\times 640\times 10\mu\text{m}$ corresponding to the interlobe, radial, HP end face
 146 and LP end face were chosen for both numerical simulations. This clearance setting was evaluated
 147 based on a genetic optimisation routine that minimises the differences between the computed and
 148 measured power and mass flow values, while closely matching the measured internal pressure curve
 149 at 2bar inlet pressure with 4,000RPM rotational speed.

150 3.1. Validation Results

151 The results from both 3D CFD and 1D chamber models agree well with the measured indicated
 152 power (Figure 6 and Table 2) at the lower rotational speeds.

Table 2. Indicated power and mass flow rates for 4,000 and 10,000RPM

	n = 4,000RPM		n = 10,000RPM	
	Power [kW]	Mass flow [kg/s]	Power [kW]	Mass flow [kg/s]
Exp	1.464	0.0450	3.445	0.0790
1D Ch. Model	1.477	0.0456	3.552	0.0809
3D CFD Model	1.442	0.0536	3.239	0.0834

153 The predicted power values from the chamber model are within 2% of the measurements
 154 ($<8,000\text{RPM}$). However, the overall results (Figure 6) clearly show that the accuracy of the numerical
 155 simulations deteriorates with increasing rotational speeds, specifically beyond 10,000RPM.

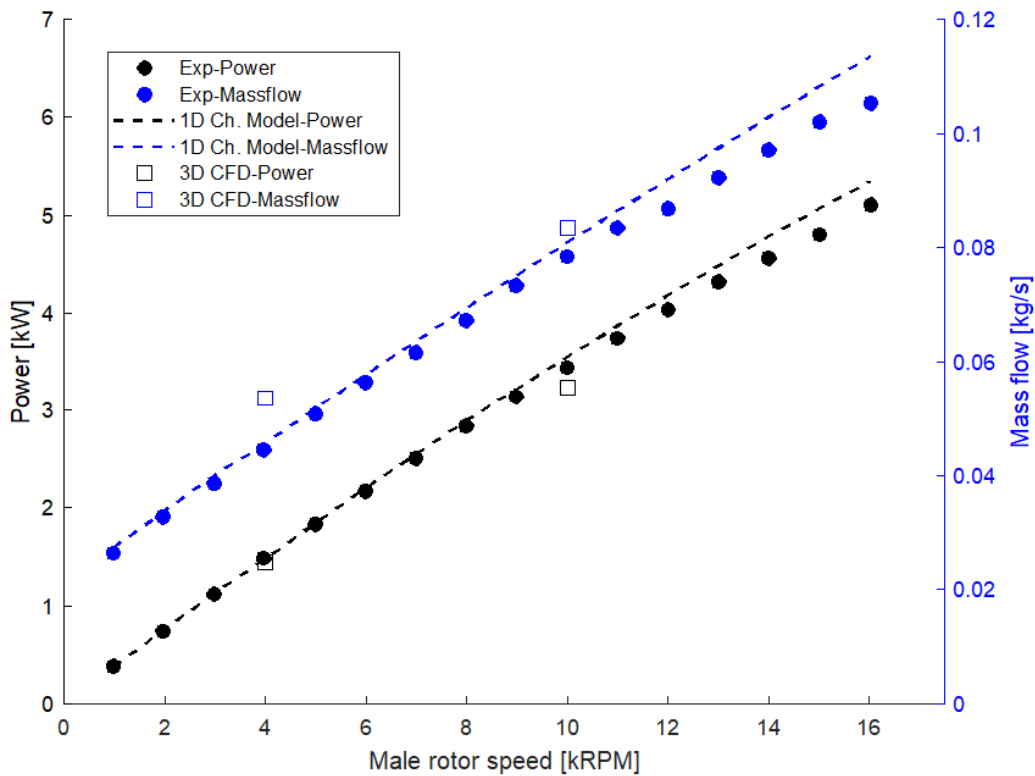


Figure 6. Measured and calculated indicated power and mass flow as a function of rotational speed [$P_i = 2\text{bar}$, $T_i = 75\text{C}$]

156 The 3D CFD model consistently under-predicts the power output and over-predicts the mass
 157 flow rates for both simulated rotational speeds, while the chamber model predicts slightly larger
 158 power output and mass flowrates. Details validation study comparing the internal pressure traces are
 159 presented in Figure 7 and 8 for the two rotational speeds shown in Table 2), which is discussed in the
 160 following section.

161 At the 4,000RPM, the CFD model significantly over-predicts the mass flow rates by 19% and
 162 under-predicts the power output by 1.5%, which results in a substantial under-prediction of the
 163 expander's specific power output (17%). The specific power output of an expander is a measure of its
 164 isentropic and mechanical efficiency and the chamber model accurately compute the specific power
 165 within 1% of the measurements. At the larger rotational speed of 10,000RPM the CFD results show
 166 better prediction of the mass flow rate and the difference with measurement is reduces to 6%.

167 The validation study is conducted using the internal pressure measurements for different
 168 rotational speeds: 4,000 (Figure 7) and 10,000RPM (Figure 8), for the inlet pressure of 2bar. The
 169 results show that both numerical models compute the indicated pressures with reasonable accuracy.
 170 The filling (up to 208 deg) and refilling (caused by net leakage of fluid into the working chamber
 171 between 250-380 deg) trends seen from the measurements are captured well with both numerical
 172 models.

173 Negligible differences are found between the chamber and high-fidelity 3D CFD models at the
 174 4,000RPM. At the higher rotational speed of 10,000RPM, the low fidelity chamber model utilizing
 175 simple orifice equations shows better prediction for the filling losses than the CFD results, at the 2bar
 176 inlet pressure.

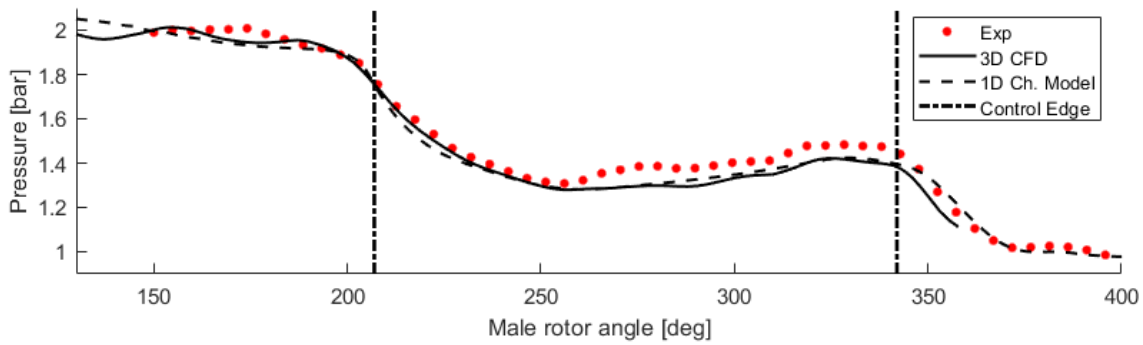


Figure 7. Validation of simulated pressure curves against male rotor's rotational angle [$n=4,000\text{RPM}$, $P_i=2\text{bar}$, $T_i=75\text{C}$]

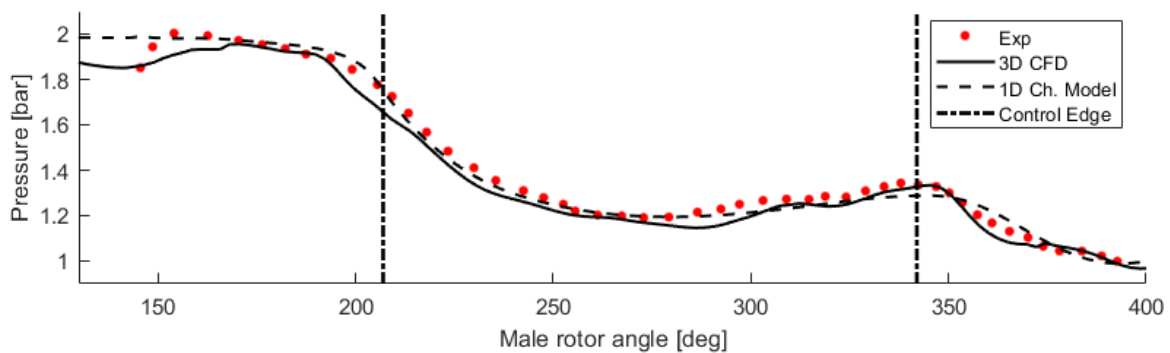


Figure 8. Validation of simulated pressure curves against male rotor's rotational angle [$n=10,000\text{RPM}$, $P_i=2\text{bar}$, $T_i=75\text{C}$]

177 Comparing the indicated diagrams for different inlet pressures at the rotational speed of
 178 10,000RPM (Figure 10) reveals that the chamber model consistently underpredicts the filling losses
 179 with increasing inlet pressures (or density). A 6% difference in filling pressure is found between the
 180 chamber model predictions and measurement, at the highest inlet pressure of 3bar. However, the results
 181 also show that refilling losses are accurately predicted with the chamber model. This suggests that
 182 despite modelling the leakages with reasonable accuracy, the orifice assumption based on isentropic
 183 nozzle relationship is insufficient to accurately capture the losses incurred via the high-pressure port,
 184 especially at the large pressure ratios (3:1).

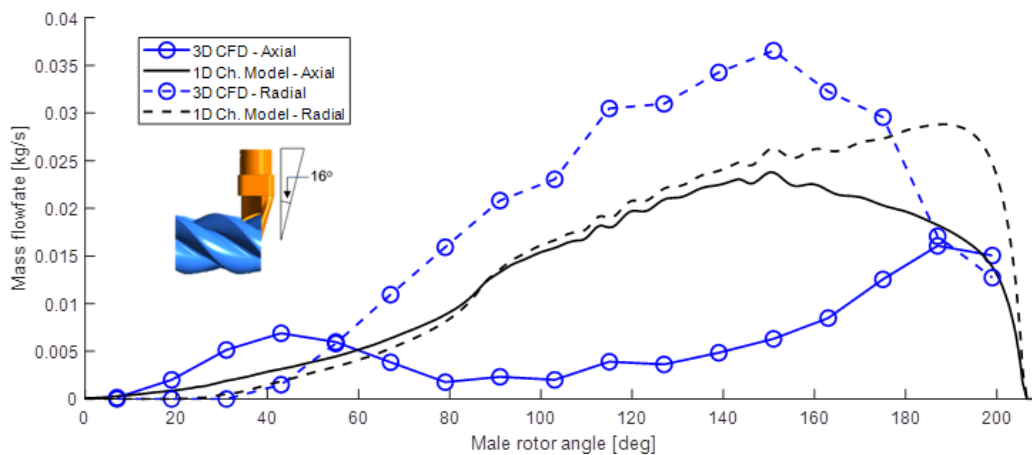


Figure 9. High pressure flow characteristics for the GL51.2-M twin screw expander [$P_i=2\text{bar}$, $n=4,000\text{RPM}$]

185 Based on the post processed results, it was clear that the two numerical models calculate
 186 significantly different flow characteristics to each other (Figure 9). The CFD model simulating the
 187 actual three-dimensional port geometry (16deg flow angle) calculates much larger flow via the radial
 188 port than the axial, while the chamber model with orifice assumption (90deg) shows similar proportion
 189 of the flow via both ports until 150deg of the male rotor position, where flow through the radial port
 190 dominates.

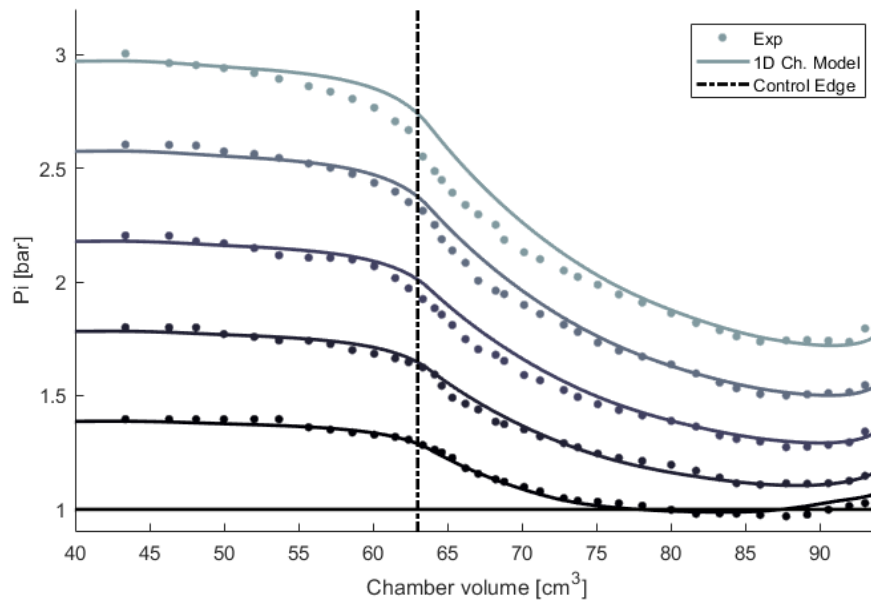


Figure 10. Validation of simulated indicated diagrams for different inlet pressure [$n=10,000\text{RPM}$, $T_i=75\text{C}$]

191 These results stress the need for an improved model for the high-pressure port. One possibility is
 192 to account for a restricted flow via the axial port based on the skewed geometry, such as using reduced
 193 port area profile based on the components of the flow directions. Improving the flow characteristics
 194 based on the 3D port geometry likely to achieve higher accuracy using the chamber model approach.

195 3.2. Maximum efficiency maps

196 The isentropic efficiency of a twin-screw expanders depends on the built-in volume ratio (ϵ_v) the
 197 actual volumetric expansion ratio of the fluid and the rotational speed. The built-in volume ratio is
 198 a function of the high-pressure port geometry, while the volumetric expansion ratio is based on the
 199 inlet and outlet fluid conditions. These two parameters determine the expanders' ability to match the
 200 expansion occurring within the machine to the required application. At higher rotational speeds the
 201 leakage become a lower proportion of the mass flow rate, resulting in higher maximum isentropic
 202 efficiency when operating with a suitable value of ϵ_v . Increasing rotational speed tends to increase
 203 the pressure drop during filling of the working chambers; this pre-expansion of the fluid can lead to
 204 optimum values of ϵ_v well below the volumetric expansion ratio for the process. Accurate modelling
 205 is therefore necessary when assessing system performance and optimum expander design.

206 Using the established Chamber model, the maximum isentropic efficiency map was evaluated
 207 using the steps below for this expander running on air:

- 208 1. Inlet pressure, P_i , is fixed
- 209 2. \dot{m} and η calculated for the range of ω and ϵ_v values
- 210 3. Maximum values of η (and corresponding values of ω and ϵ_v) identified as a function of \dot{m}
- 211 4. Repeat steps 1-3 across the range of P_i values
- 212 5. Calculated data allows contour plots of maximum η and corresponding ϵ_v and ω values as
 213 functions of P_i and \dot{m}

214 The range of values considered for the input parameters was; $1 \leq \epsilon_v \leq 10$ in steps of 0.5, $500 \leq \omega \leq$
 215 $16,000$ RPM in steps of 500 RPM, and $1.5 \leq P_i \leq 3$ bar in steps of 0.25 bar. A constant outlet pressure
 216 of 1 bar was used in all cases. The resulting contour maps are shown in Figures 11-13.

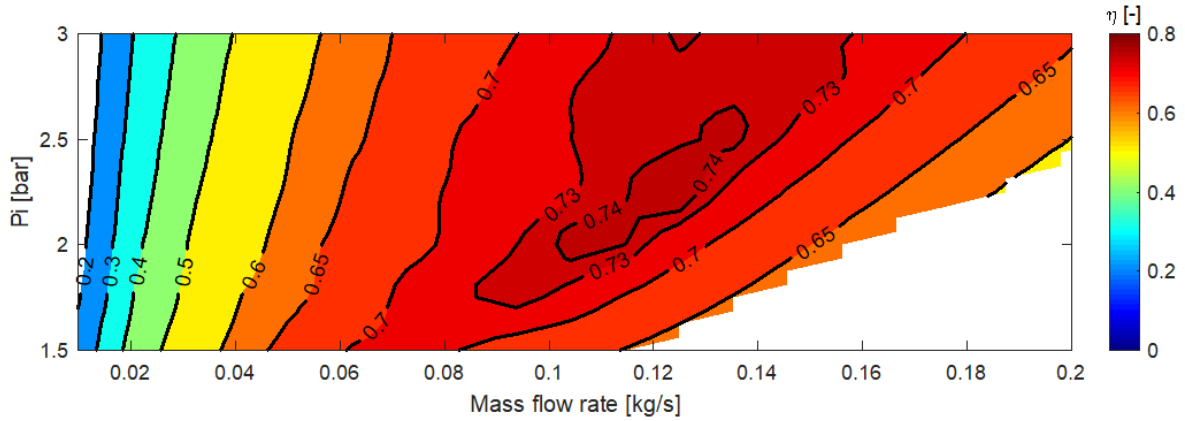


Figure 11. Maximum efficiency map for GL51 twin-screw expander running on air [$T_i=75\text{C}$, $P_o=1\text{bar}$]

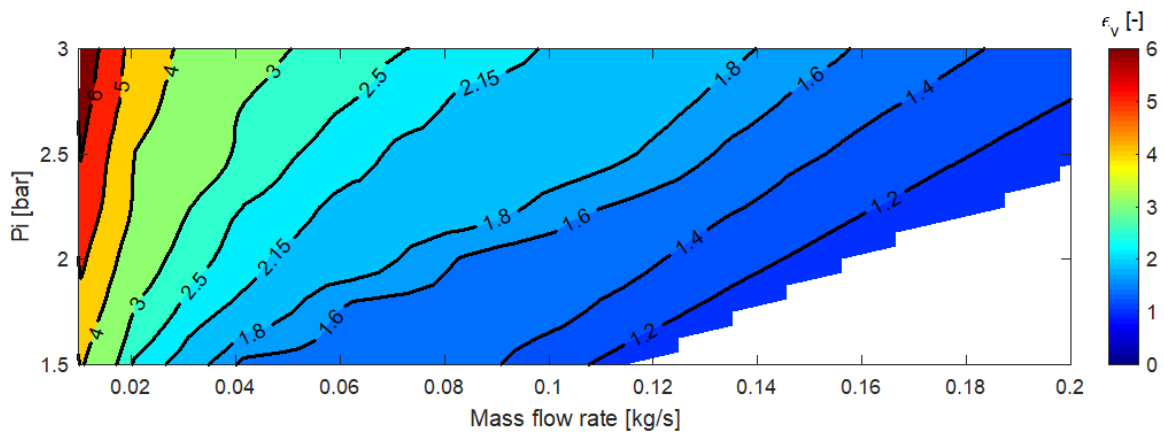


Figure 12. Built-in volume ratio (ϵ_v) corresponding to maximum isentropic efficiency of GL51 twin-screw expander running on air [$T_i=75\text{C}$, $P_o=1\text{bar}$]

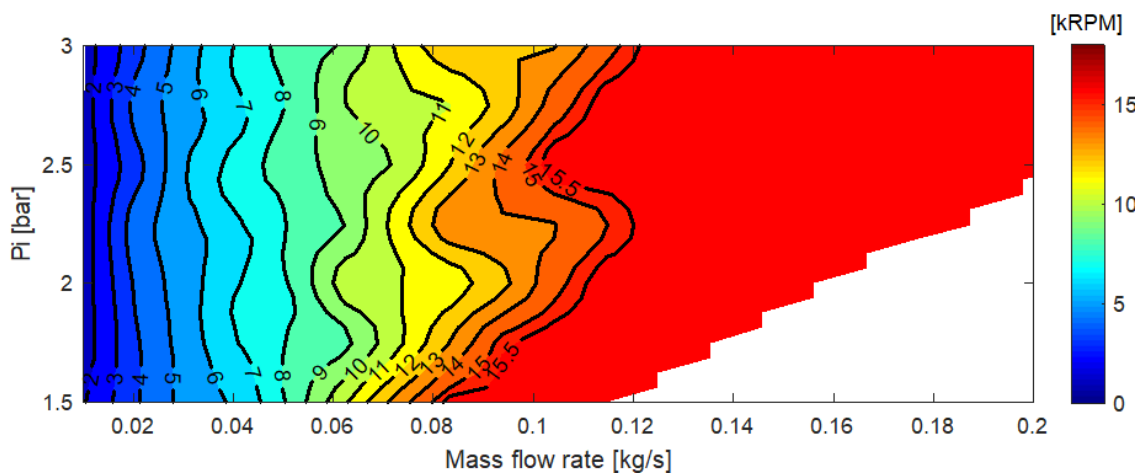


Figure 13. Rotational speeds corresponding to maximum isentropic efficiency of GL51 twin-screw expander running on air [$T_i=75\text{C}$, $P_o=1\text{bar}$]

217 Based on the results (Figure 11), the better efficiency operation is achieved with increasing mass
218 flow rates up to 0.07kg/s for all investigated inlet pressures. The global optimum efficiency is achieved
219 at mass flow rates between 0.100-0.140kg/s with inlet pressures of 2.1-2.6bar respectively. This range
220 of operation with maximum efficiency is achieved with a close to constant volume ratio of $\epsilon_v = 1.6$
221 (Figure 12) for rotational speeds above 15,500RPM (Figure 13). Larger mass flow rates beyond 0.14kg/s,
222 shows reduction in maximum efficiency. The losses during filling meaning that the pressure at the
223 start of expansion is relatively low, which effectively reduces the work done (area of the pV diagram),
224 resulting in less mass per cycle and less work per cycle. The pressure drop across the inlet port means
225 that there is lost work, and so specific work tends to decrease at higher speeds.

226 For the conditions above the 15,000RPM, the experimented machine configuration with ϵ_v of
227 1.47 was found to be operating close to the best conditions suggested by the maximum efficiency
228 maps. At the experimented condition with inlet pressure of 2bar and mass flow rate of 0.102kg/s, the
229 experimentally established isentropic efficiency was found to be 0.7, while the optimum operation
230 recommended by the efficiency map (Figure 11) for 2bar inlet pressure with 0.102kg/s is with $\epsilon_v=1.49$
231 where the machine achieves an isentropic efficiency of 0.74.

232 4. Conclusions

233 Positive displacement machines have been identified as appropriate expanders for small scale
234 power generation systems such as ORCs. Detailed understanding of the fluid expansion process is
235 required to optimise the machine design and operation for specific applications, and accurate design
236 tools are therefore essential.

237 Using experimental data for air expansion, both CFD and chamber models have been applied
238 to investigate the numerical accuracy on the power output and mass flowrate. A detailed validation
239 study was conducted using the measured internal pressure curves to assess the leakage and the filling
240 loss predictions. Both models are shown to predict pressure variation and power output with good
241 accuracy. However, results also indicates that the accuracy of the numerical predictions deteriorates
242 with increasing rotational speeds and increasing inlet densities. These finding suggests that further
243 investigations are required to quantify and assess the simple orifice assumption considered for leakage
244 and filling loss predictions. Nevertheless, the validated chamber model has been successfully used to
245 demonstrate the process of determining the optimum built-in volume ratio and rotational speed for
246 the experimented conditions.

247 An extension of this work validating two-phase R245fa expansion is published at the Rankine2020
248 conference [17].

249 **Author Contributions:** Conceptualization, K.V., M.R. and A.K.; methodology, K.V. and M.R.; validation, K.V.;
250 formal analysis, K.V.; investigation, K.V.; resources, A.K.; data curation, K.V.; writing–original draft preparation,
251 K.V.; writing–review and editing, K.V., M.R. and A.K.; visualization, K.V.; supervision, M.R. and A.K.; All authors
252 have read and agreed to the published version of the manuscript.

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256 **Conflicts of Interest:** The authors declare no conflict of interest.

257 Abbreviations

258 The following abbreviations are used in this manuscript:

259	Exp	Experimental
260	1D Ch. Model	One dimensional chamber model
	3D CFD Model	Three dimensional computational fluid dynamics model

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300 **Sample Availability:** Samples of the compounds are available from the authors.

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