SCORG™ – Tutorial: Thermodynamic module for performance analysis of screw expanders

SCORG™ is the unique design platform for rotary twin screw machines. The tool includes modules for designing and editing rotor profiles, executing a basic thermodynamic calculation based on quasi 1D chamber models and generating the deforming working chamber grids for selected commercial CFD solvers. For more information on the product please visit the website: www.pdmanalysis.co.uk or refer to documentation help.

This tutorial lists the steps for setting up and performing Thermodynamic calculation for performance analysis of screw expanders The user is expected to be familiar with principle of operation and modelling of screw machines. It is highly recommended that the users who attempt this tutorial study the books on the performance prediction methods for screw compressors[1 2]. This Tutorial should be studied alongside the SCORG™ User Manual and SCORG™ Thermodynamic module tutorial.

The steps explained in this tutorial are demonstrated for Windows 10, x64 bit OS. Refer to SCORG™ Installation Guide V2022 for the system and hardware requirements.

Table of Contents

[1] N. Stosic, I.K. Smith, A. Kovacevic Screw Compressor Mathematical Modelling and Performance Calculation, Springer, UK 2005, ISBN-10 3-540-24275-9

[2] A. Kovacevic. N. Stosic, I.K. Smith, Screw Compressor Three Dimensional Computational Fluid Dynamics and Fluid Solid Interaction, Springer, 2006, ISBN 3-540-36302-5

1 Introduction

Screw expanders and compressors are rotary positive displacement machines. They can be oil free or oil injected. Oil free machines have their rotors synchronised by the additional pair of timing gears attached to rotor shafts in order to maintain the contact free operation. In the oil injected screw machines, one rotor drives the other through direct contact, Figure 1.1.

The screw machine rotors are helically lobed gears with special rotor profile. Together with the casing they form a closed interlobe space called the working chamber which changes the size and shape during the operation of the machine. The working chamber itself is periodically connected to the suction and discharge chambers through ports with flow areas changing in time both in shape and size. The schematic view of a screw machine (compressor, pump or an expander) is shown in Figure **1.2**.

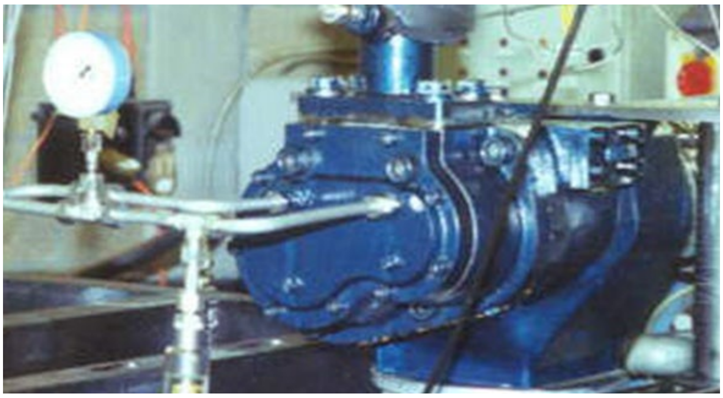


Figure 1.1 Oil injected twin screw expander

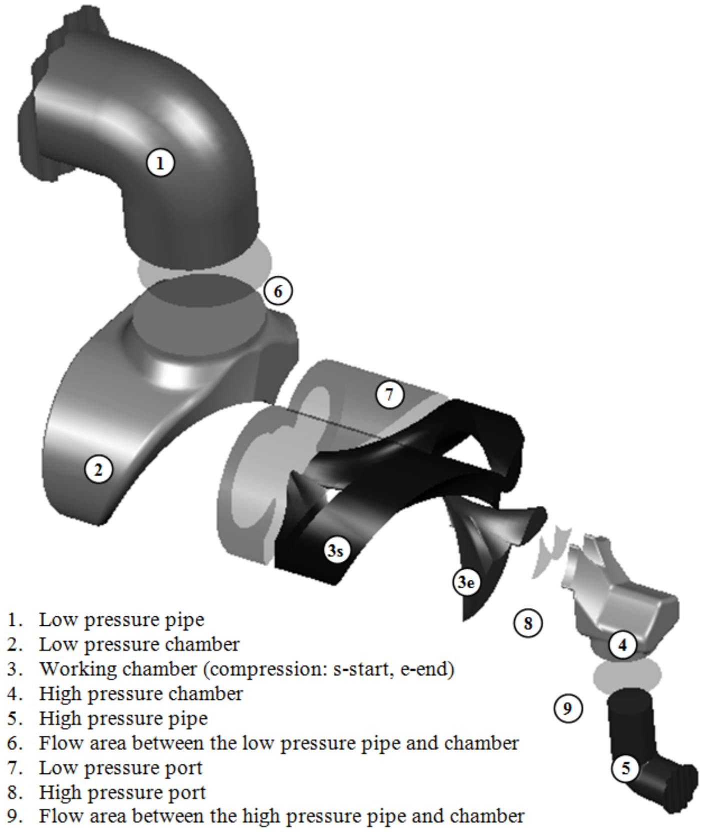


Figure 1.2 Configuration of a screw compressor or expander

Chamber modelling of screw machines is well established methodology. It assumes that all thermodynamic values, such as the pressure, temperature, density etc. are uniform within the respective control volume. Any of the control volumes can be considered as open thermodynamic systems, which exchange fluid mass and energy with the environment, as shown in Figure 1.3. The mass and energy flows, in and out of the control volume affect the quantity of mass and internal energy of the fluid inside the working chamber. The rate of change of mass and energy within the working chamber are defined by the conservation laws of mass and energy respectively expressed in the form of differential equations. Other phenomena within a control volume and at its boundaries are modelled by a number of algebraic equations which describe leakage, inlet and outlet fluid velocities, oil injection and heat exchange with environment and oil. The model is closed by the equation of state of the working fluid which can be defined as either an ideal or real gas.

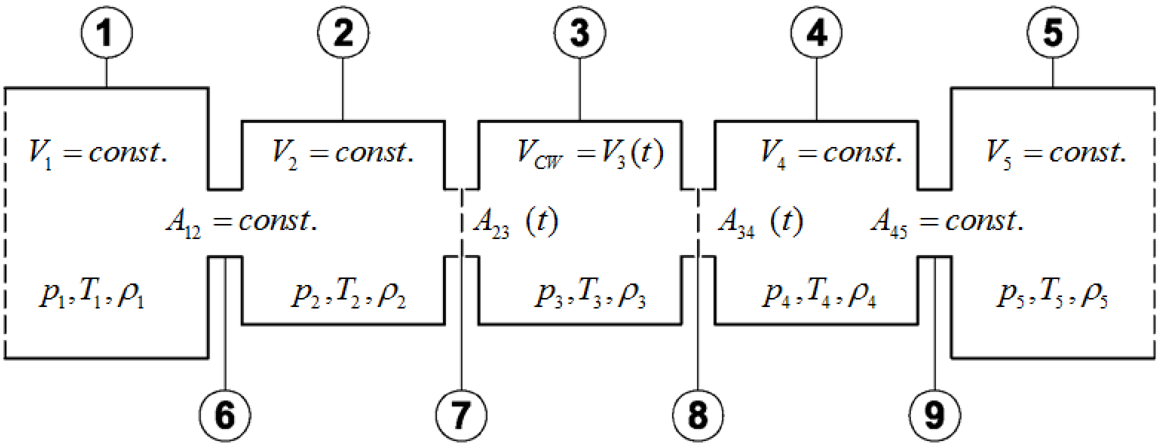


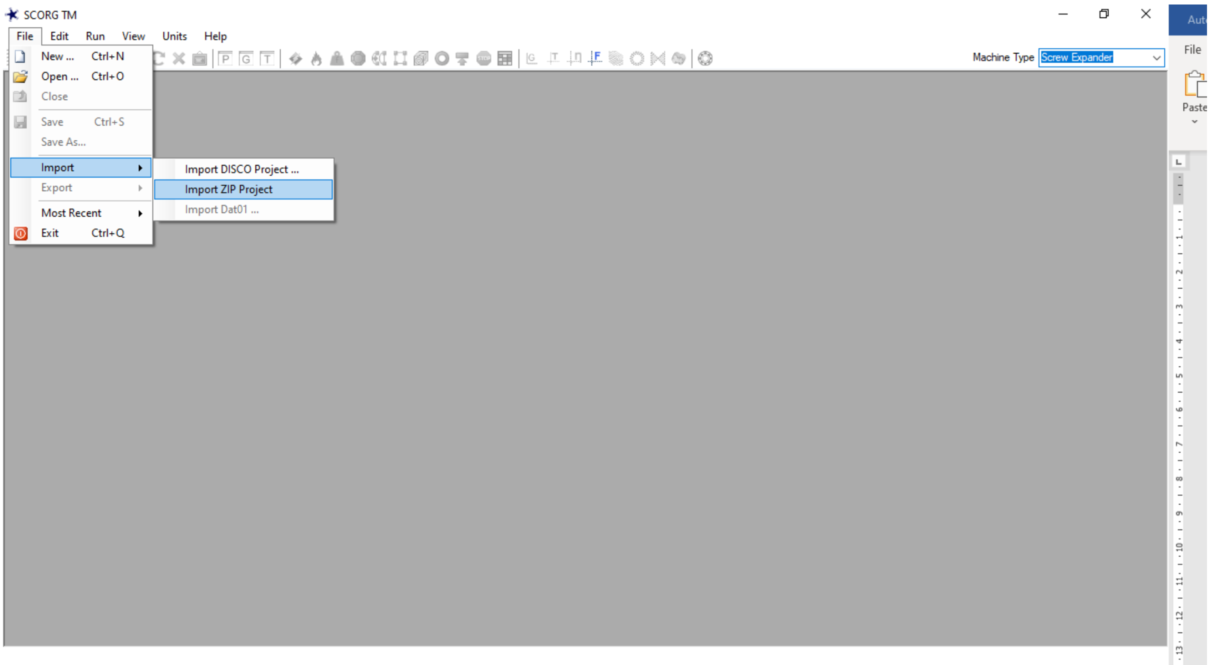
Figure 1.3 Schematic view of a screw machine chamber configuration

This Tutorial will provide a step by step guide to setup and execute thermodynamic simulation of a typical twin screw expander. Two examples are presented in this tutorial. The first is the dry air screw expander with 3/5 lobe combination and the second one is the screw expander with 4/5 lobes operating on refrigerant R245fa in an ORC system.

2 Oil free air screw expander

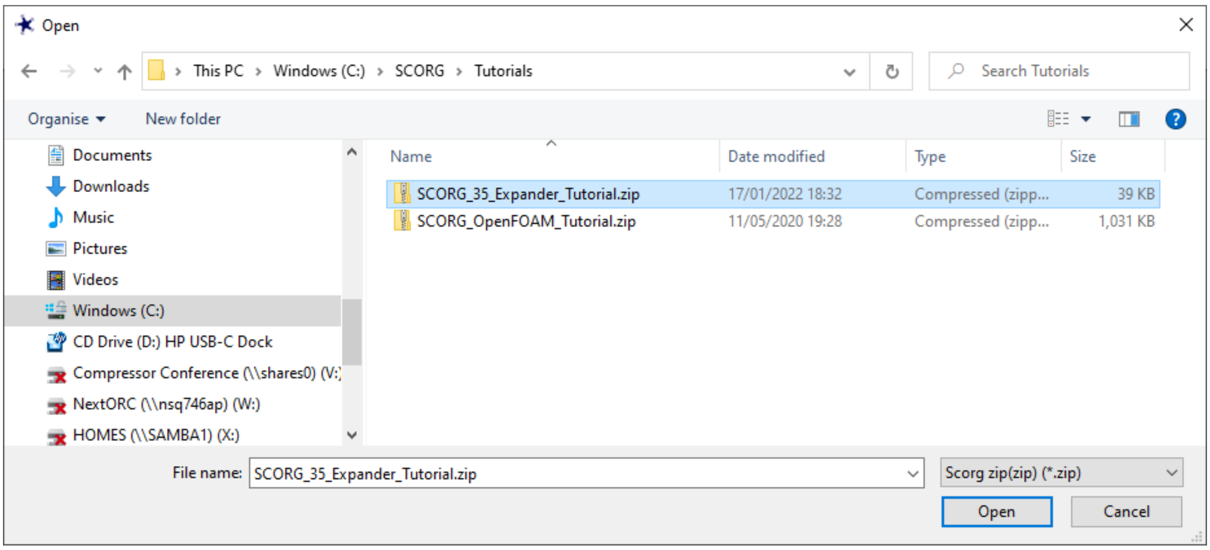
Start SCORG™ Project

- Launch SCORG™ on the Desktop.
- Select File → Import → Import ZIP Project



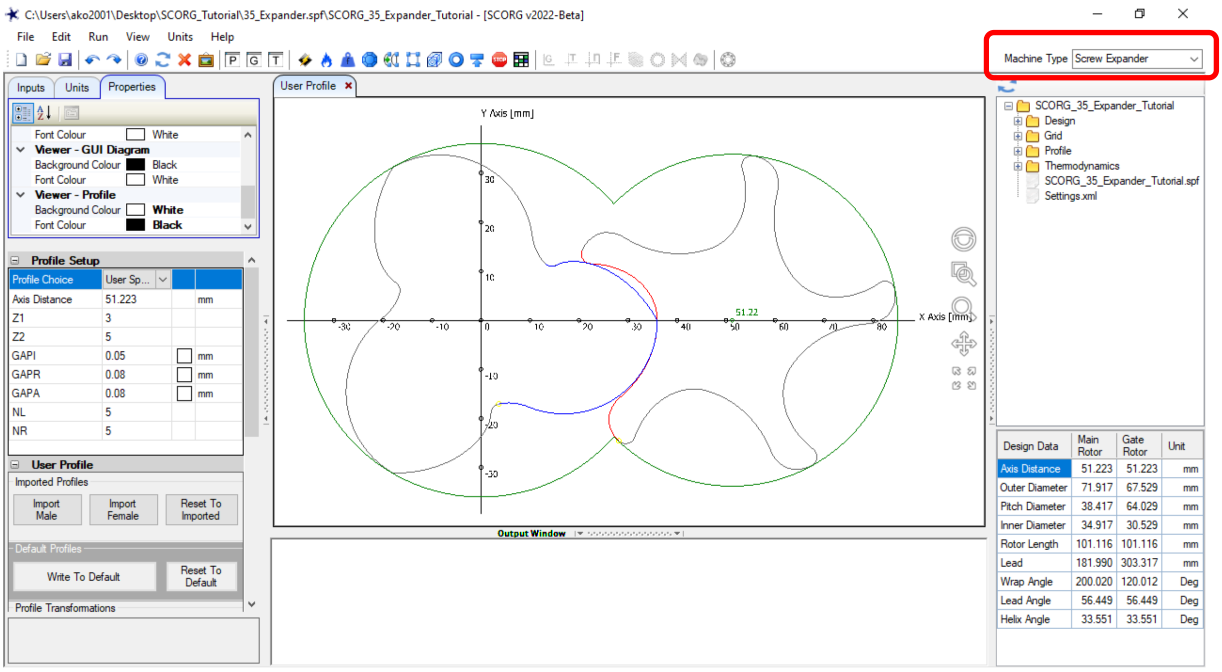
- Select SCORG_35_Expander_Tutorial.zip from C:\SCORG\Tutorial folder and click Open.

- Save the project in a new folder named SCORG_Thermodynamics→ SCORG_Thermodynamics_Tutorial.spf



Save the project under the name 35_Expander.spf.

- The GUI of SCORG™ in the figure bellow shows the mains items of the front panel.



The case you imported from .zip archive is 3/5 expander with the main rotor diameter of 71.917 mm, relative rotor length L/D=1.401. We will simulate this machine as an air expander at the variety of inlet pressures from 2 to 4 bar expanding to atmosphere.

Firstly, set the operating conditions in the Thermodynamics->Working conditions to the values shown below and ensure the working fluid is air and the oil injection is switched Off.

Working Conditions

Wtip	45.1869	m/s
Rotor Speed	12000	RPM
P0	1	bar
Pr	2	bar
T0	20	℃
Tr	80	℃
Tevp	-4.99	℃
Tcond	40.01	℃
T Ambient	19.85	℃
Include heat transfer	No	
X	1	

Working Fluid

Fluid	Ideal ...	
Gamma	1.4	
RGas	287	J/(kg.K)
Z	1	

Fluid Injection

Fluid Injection	Off	
P	3	bar
T	36.85	℃
Injection Angle	68.755	Deg
Axial Position	100	mm
Port Diameter	8	mm
Doil	0.01	mm
CpOil	2050	J/(kg.K)
ρ	950	kg/m³
Viscosity of Oil	5E-06	m²/s

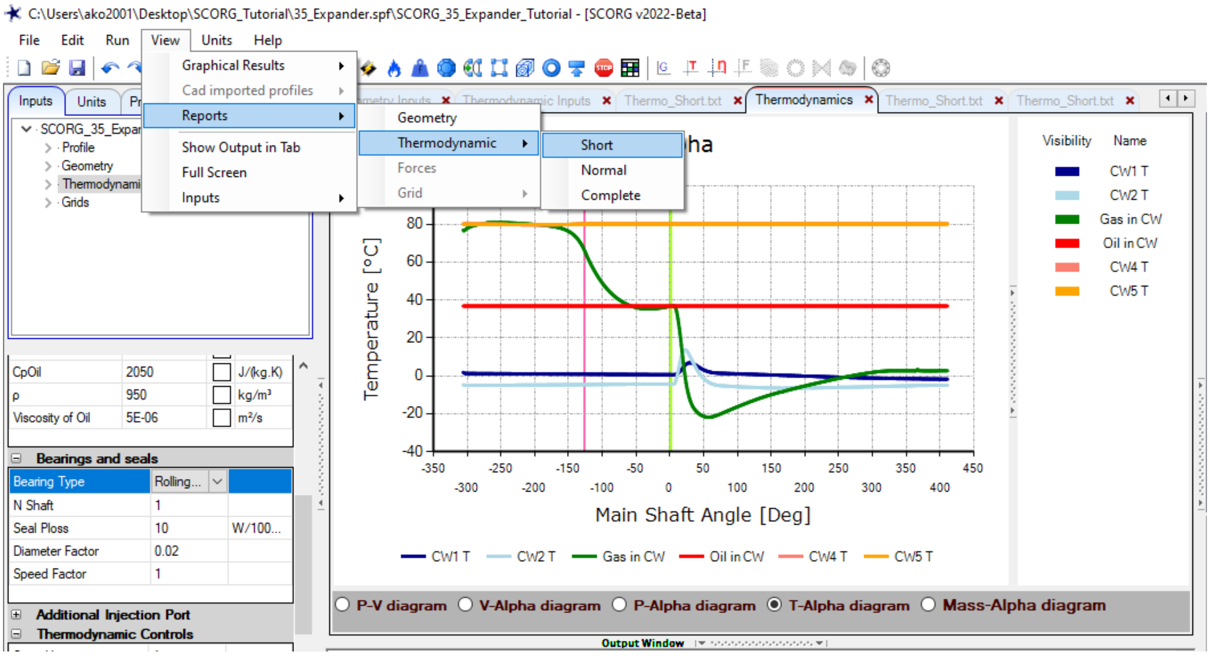
Then adjust the Thermodynamic Controls to the values shown below.

Thermodynamic Controls

Speed loop	4	
Psuc loop	1	
Pdis loop	3	
Convergence loop	10	
Convergence criteria	1	℃
ΔWtip	7.5312	m/s
ΔPsuc	0	bar
ΔPdis	1	bar
ΔTevp	5	℃
ΔTcon	5	℃
Clearance adjustment	No	
Short report settings	Settings...	
Thermodynamic solver	SCORG	

Ensure that the Machine Type selected in the top right corner of the screen is “Screw Expander”.

In this case we will calculate performance map of this air expander for 4 different speeds from 12000 – 18000 and 3 different inlet pressures from 2 – 4 bar.
Press Thermodynamic calculate button. The calculation of the performance map will take couple of minutes.
The results could be viewed in tabular form using short report as shown below



The result of calculation is:

SCORG - Thermodynamic Performance Calculation

Date: 17/01/2022 22:33:48

Gas properties - Ideal gas
Cp/Cv = 1.4
R = 287 J/kgK Z = 1

Machine: Expander
Lobe combination : 3/5
Size : 72/141 14
Mechanical seals : 1

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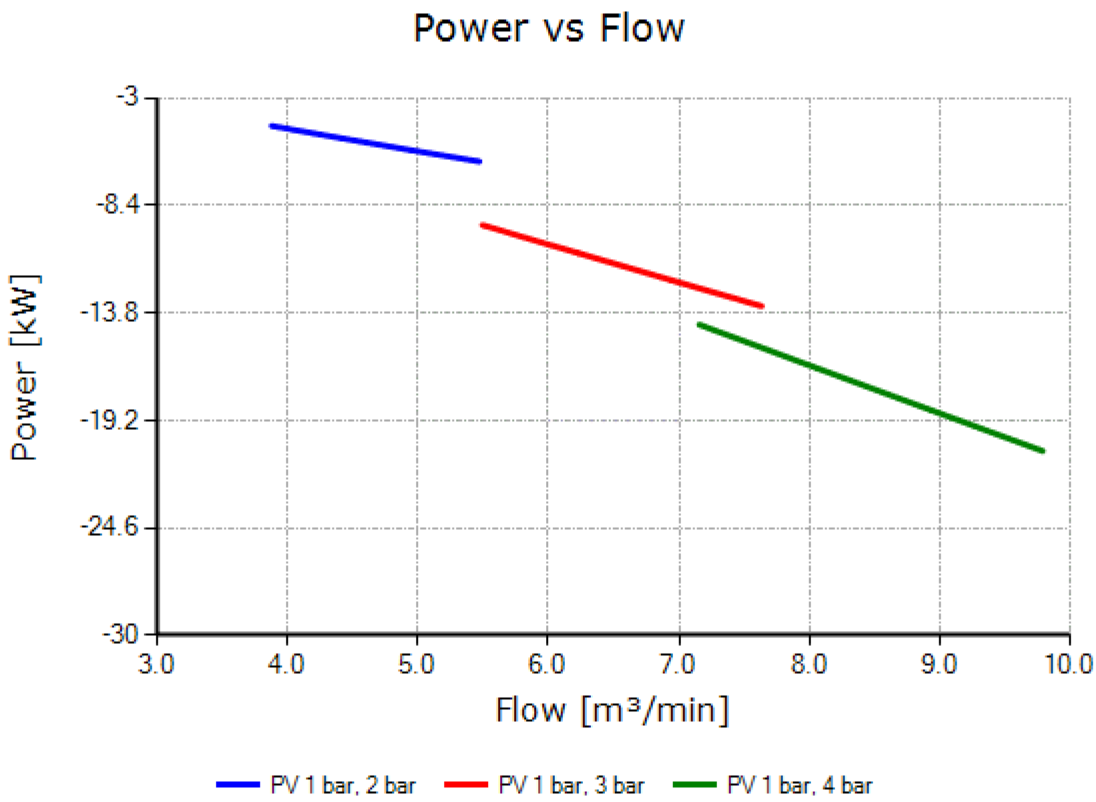
WTP m/s	N RPM	Q m3/m	Qn nm3/m	M kg/min	ηv _	Power Kw	Psp kW/m3/min	ηad _	P1 bar	T1 degC	P2 bar	T2 degC
45.19	11999.9	3.873	3.641	4.327	1.1295	-4.386	1.132	0.8863	1	38.721	2	80.01
52.72	13999.9	4.416	4.174	4.961	1.1039	-5.012	1.135	0.8882	1	37.053	2	80.01
60.25	15999.9	4.948	4.695	5.58	1.0822	-5.607	1.133	0.887	1	35.855	2	80.01
67.78	17999.8	5.47	5.204	6.185	1.0634	-6.173	1.128	0.8833	1	35.005	2	80.01
45.19	11999.9	5.493	5.461	6.491	1.6017	-9.371	1.706	0.7932	1	21.688	3	80.01
52.72	13999.9	6.222	6.261	7.442	1.5552	-10.775	1.732	0.8051	1	18.158	3	80.01
60.25	15999.9	6.935	7.043	8.372	1.5168	-12.133	1.75	0.8134	1	15.5	3	80.01
67.78	17999.8	7.634	7.808	9.281	1.4841	-13.444	1.761	0.8187	1	13.474	3	80.01
45.19	11999.9	7.155	7.281	8.655	2.0865	-14.374	2.009	0.7086	1	14.915	4	80.01
52.72	13999.9	8.056	8.348	9.922	2.0136	-16.553	2.055	0.7248	1	9.754	4	80.01
60.25	15999.9	8.935	9.391	11.162	1.9541	-18.67	2.09	0.7371	1	5.774	4	80.01
67.78	17999.8	9.794	10.41	12.373	1.9041	-20.725	2.116	0.7464	1	2.658	4	80.01

The results can be also shown in graphical form of performance map by selecting performance map button:

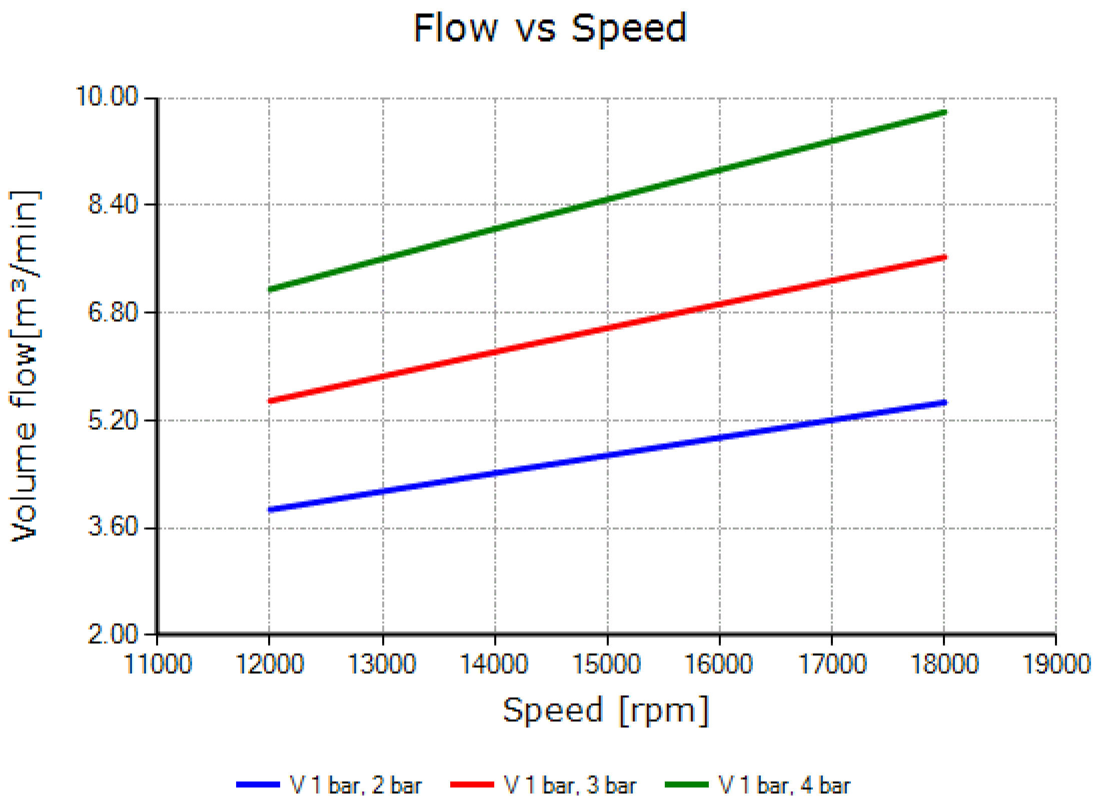
Number of diagrams can be generated directly in scorg including Power vs. Flow diagram shown below



Other diagrams which can be directly generated in SCORG are listed below

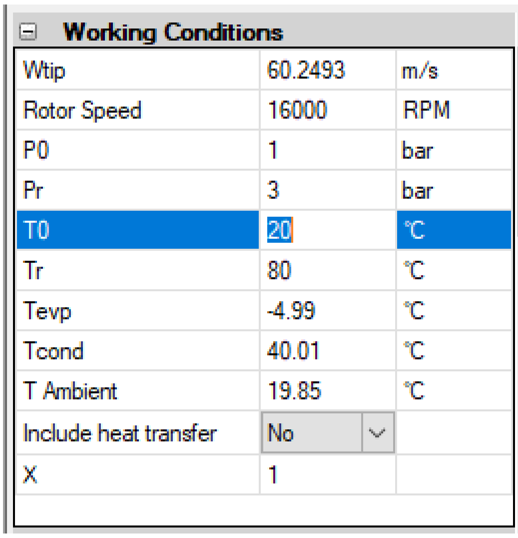
Please note, since this is an expander it will generate power which is indicated with a negative value opposite to a compressor which consumes power and its value will be positive.

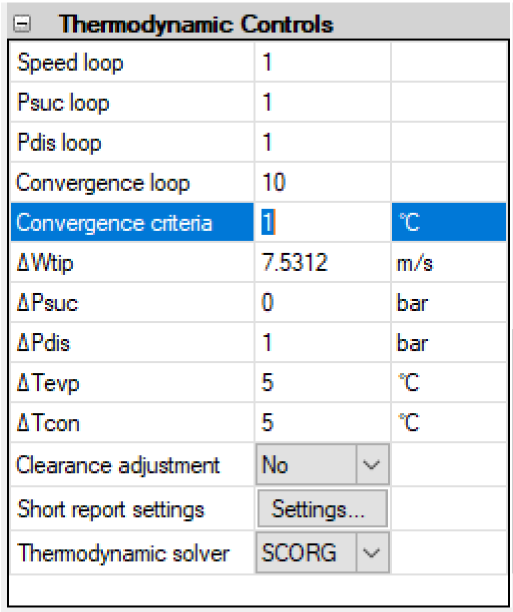
Higher inlet pressures and higher speeds will generate higher power but they will also mean the increased flow rate as shown in the diagram below.



Diagrams can be directly exported from SCORG by selecting options form the menu which can be obtained by clicking the right mouse button while the cursor is on the diagram:

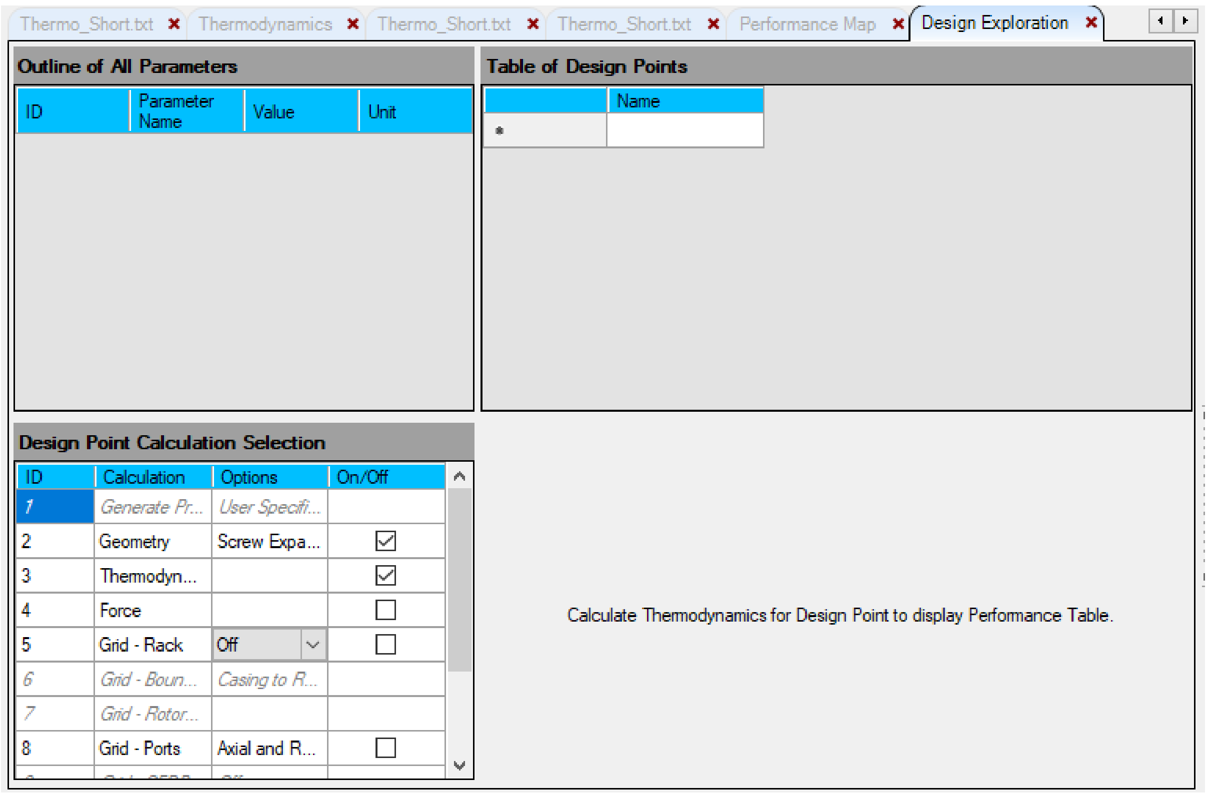
To explore the influence of clearances on the performance of a screw expander, one can use design exploration feature introduced in SCORG 2022. Firstly, select a single speed and pressure loop and Working conditions as shown below.



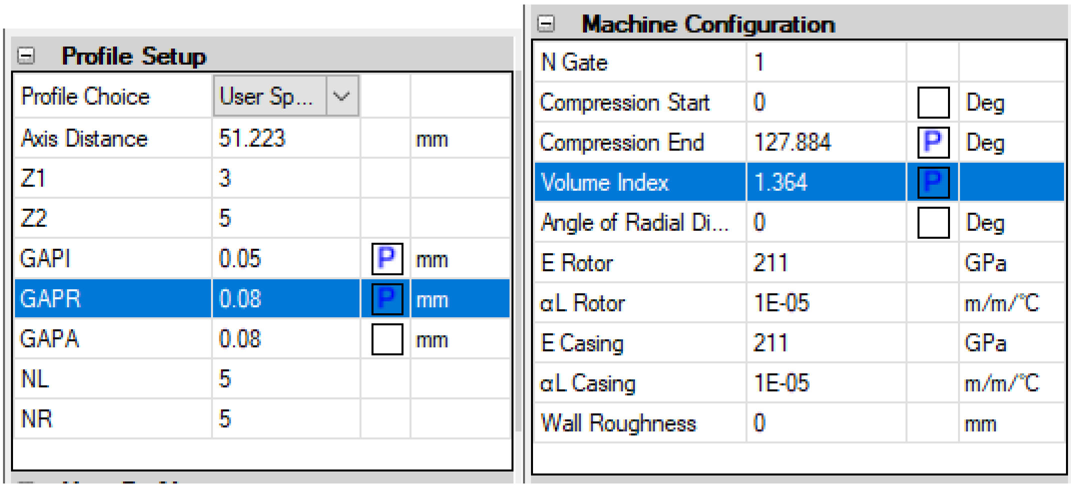


Select Design Exploration button as shown in the snapshot below.

This will open Design Exploration menu in the main SCORG window as shown below:

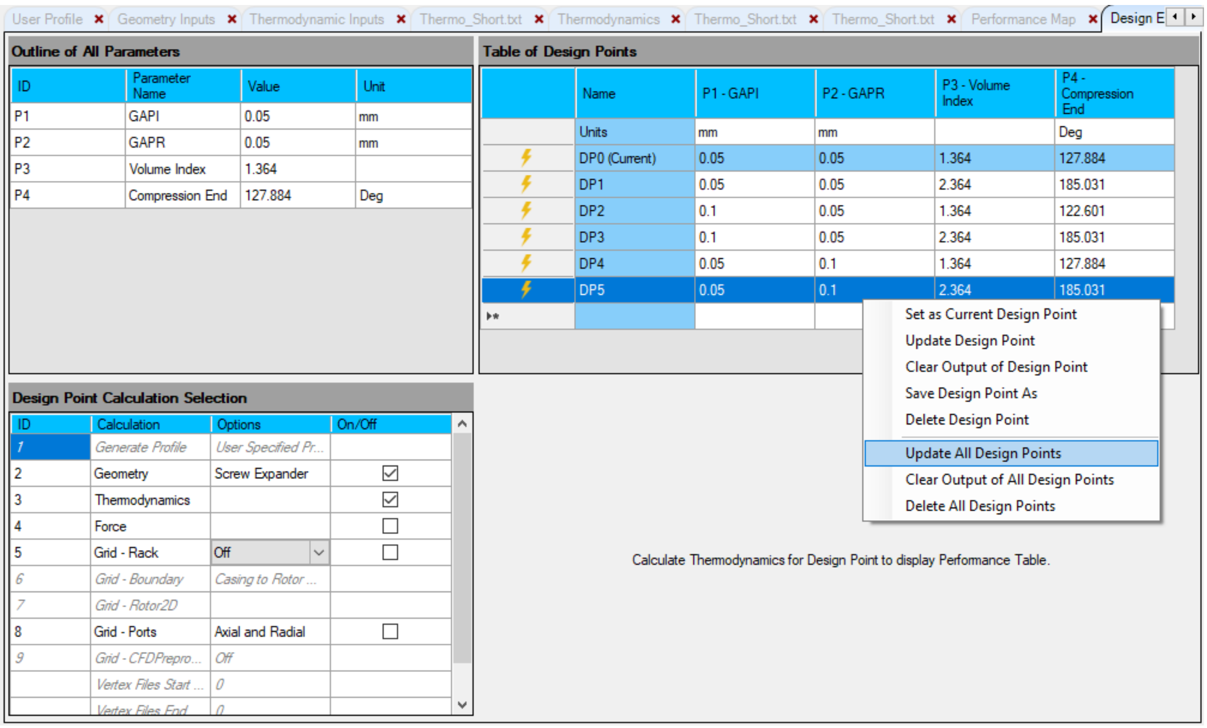


Select parameters of interest for Design exploration. In this case, we will select interlobe and radial clearances in profile setup and volume index in Machine configuration as shown below

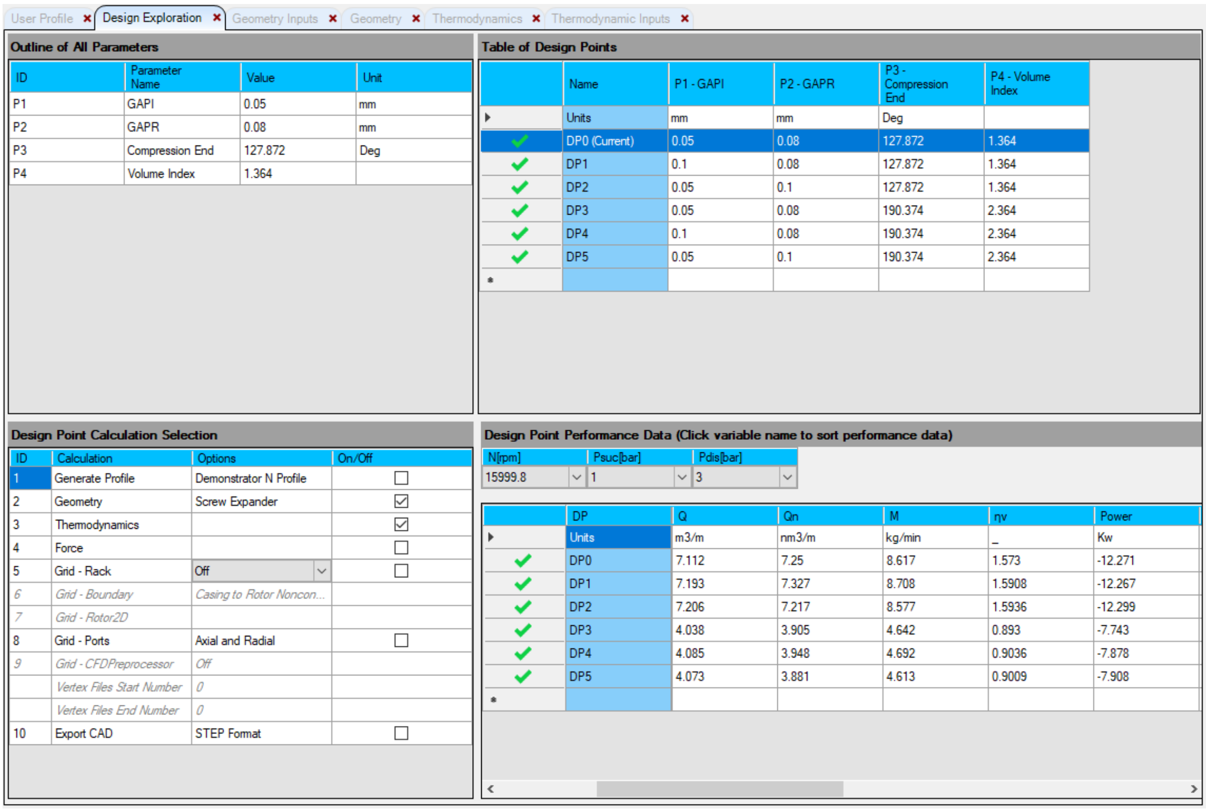


Details on how to use Design exploration menu are available in the Help manual and in the Design exploration Tutorial available in the SCORG library (C:\SCORG\User Manual and C:\SCORG\Tutorials)

Select desired combination of parameters to explore and required calculation procedures to be performed as shown in the snapshot below



Then click right mouse button on any of the design points and select option Update All Design Points. Once finished, the overview of results for selected design points is given in the bottom right window of the Design Exploration tab, as shown in the figure below..



User Profile | Design Exploration | Geometry Inputs | Geometry | Thermodynamics | Thermodynamic Inputs

Outline of All Parameters

ID	Parameter Name	Value	Unit
P1	GAPI	0.05	mm
P2	GAPR	0.08	mm
P3	Compression End	127.872	Deg
P4	Volume Index	1.364	

Table of Design Points

	Name	P1 - GAPI	P2 - GAPR	P3 - Compression End	P4 - Volume Index
	Units	mm	mm	Deg	
✓	DP0 (Current)	0.05	0.08	127.872	1.364
✓	DP1	0.1	0.08	127.872	1.364
✓	DP2	0.05	0.1	127.872	1.364
✓	DP3	0.05	0.08	190.374	2.364
✓	DP4	0.1	0.08	190.374	2.364
✓	DP5	0.05	0.1	190.374	2.364

Design Point Calculation Selection

ID	Calculation	Options	On/Off
1	Generate Profile	Demonstrator N Profile	☐
2	Geometry	Screw Expander	☑
3	Thermodynamics		☑
4	Force		☐
5	Grid - Rack	Off	☐
6	Grid - Boundary	Casing to Rotor Noncon...	
7	Grid - Rotor2D		
8	Grid - Ports	Axial and Radial	☐
9	Grid - CFDPreprocessor	Off	
	Vertex Files Start Number	0	
	Vertex Files End Number	0	
10	Export CAD	STEP Format	☐

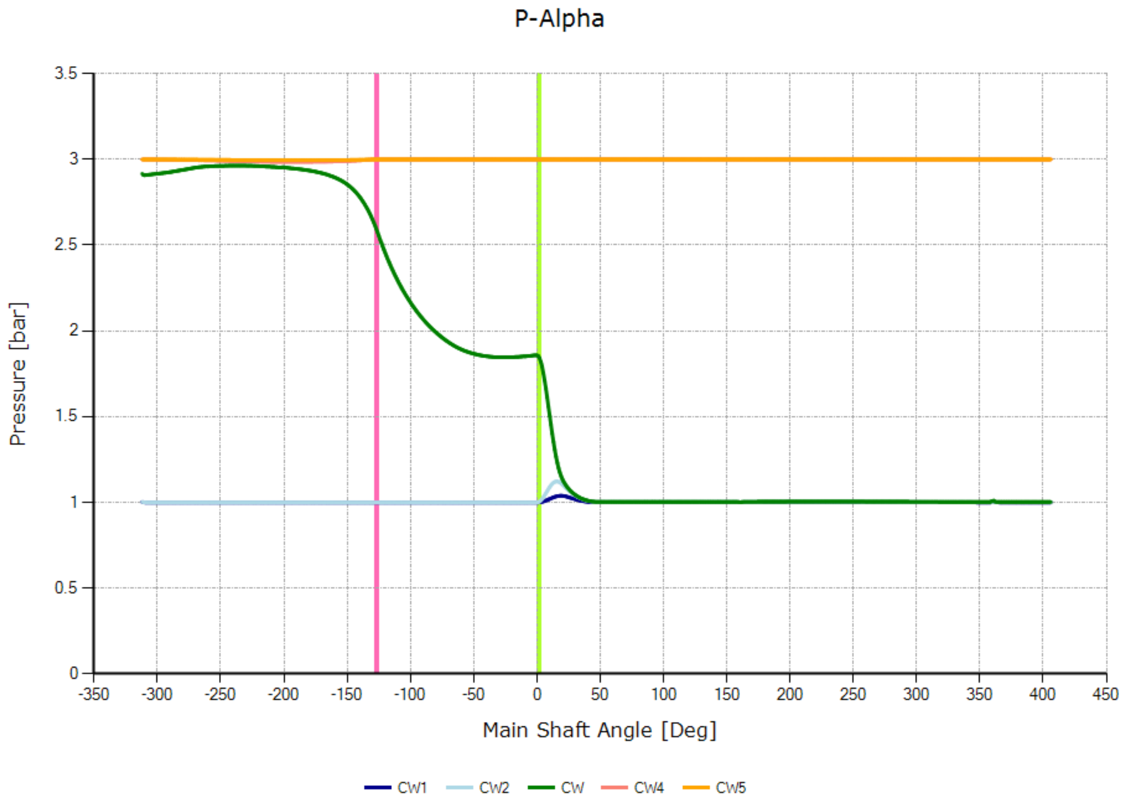
Design Point Performance Data (Click variable name to sort performance data)

N[rpm]	Psuc[bar]	Pdis[bar]
15999.8	1	3

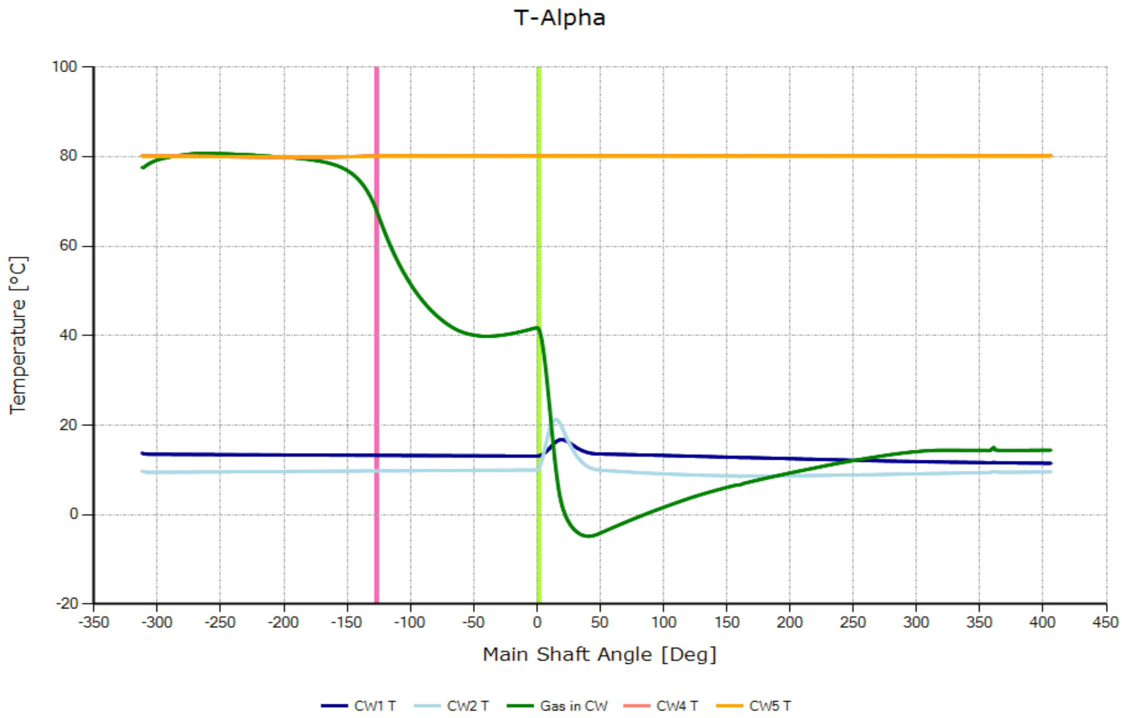
	DP	Q	Qn	M	ηv	Power
	Units	m3/m	nm3/m	kg/min	_	Kw
✓	DP0	7.112	7.25	8.617	1.573	-12.271
✓	DP1	7.193	7.327	8.708	1.5908	-12.267
✓	DP2	7.206	7.217	8.577	1.5936	-12.299
✓	DP3	4.038	3.905	4.642	0.893	-7.743
✓	DP4	4.085	3.948	4.692	0.9036	-7.878
✓	DP5	4.073	3.881	4.613	0.9009	-7.908

It is worth mentioning that higher power output is achieved with larger radial clearances and lower Volume index value, which means larger high-pressure port.

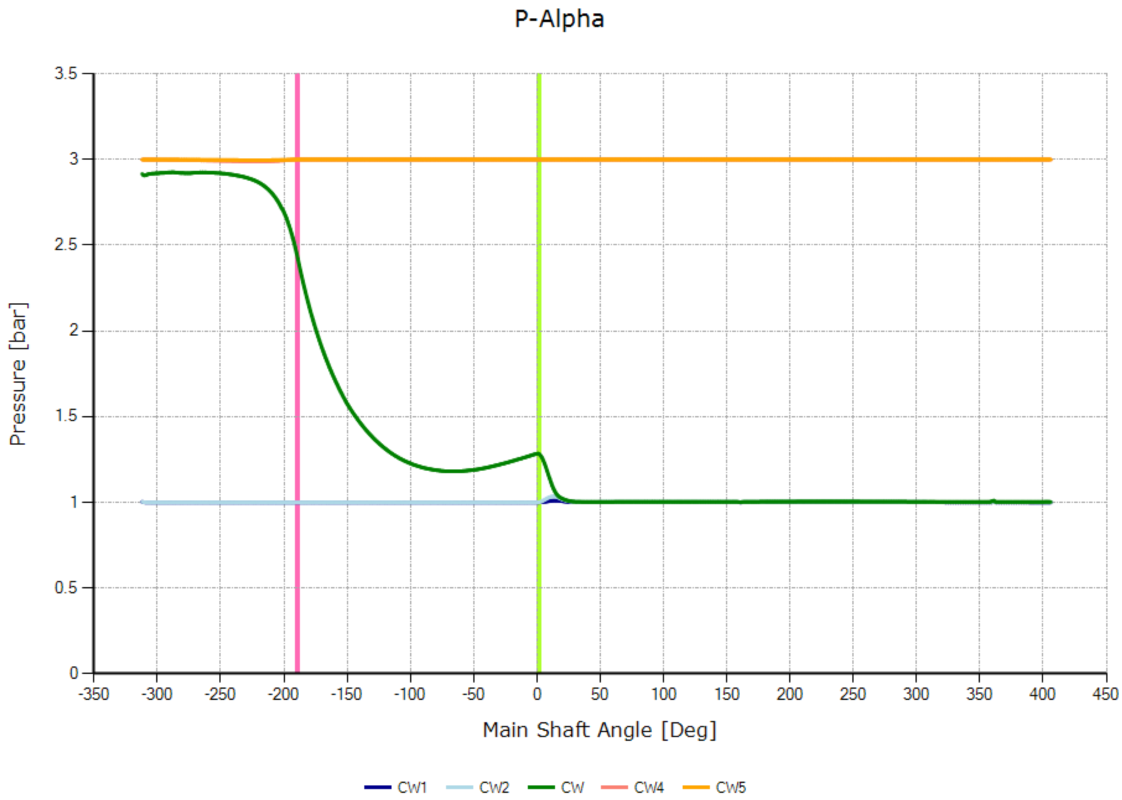
To examine individual cycle diagrams, it is necessary to set a Current Design Point. In the above figure, DP0 is Current Design Point The pressure cycle diagram is shown below.



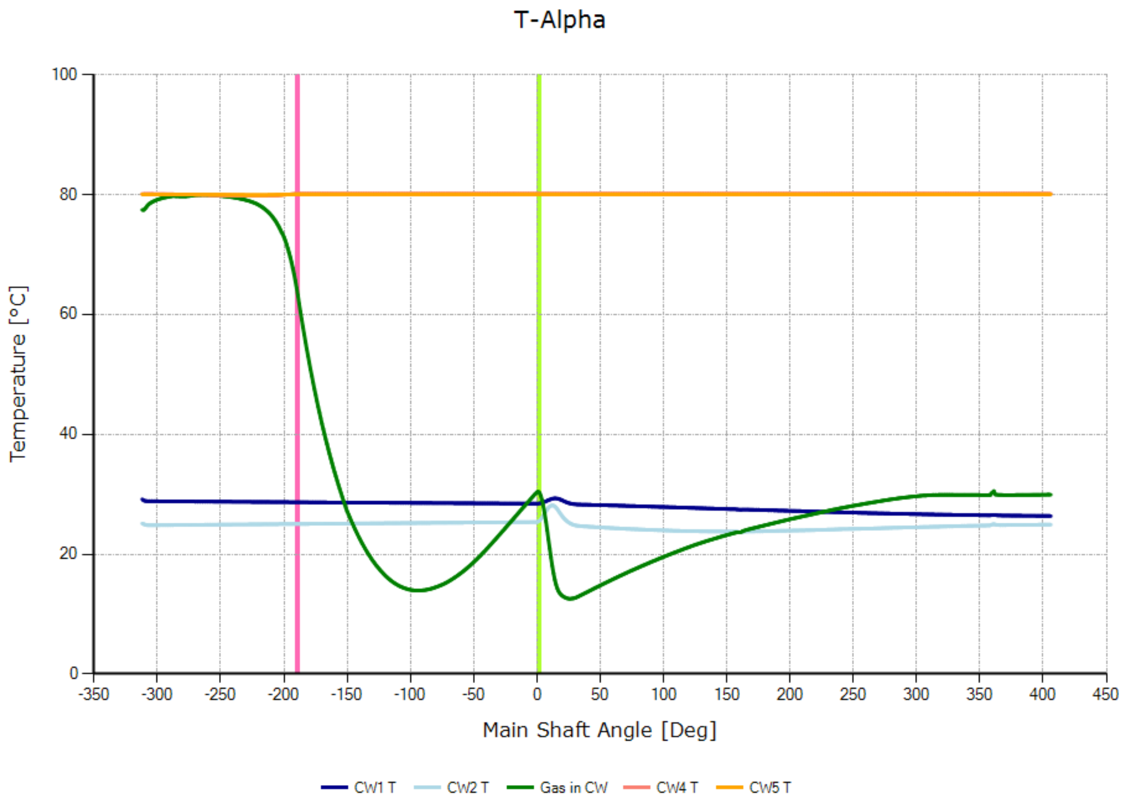
Corresponding Cycle temprature is shown below



To set DP3 as Current Design Point, click the right mouse button anywhere on the line of DP3 and choose: ”Set as Current Design Point”. This will update the pressure diagram for this design point as shown below.



The corresponding cycle temperature for DP3 is shown below.



In the case of DP3, due to the reduced size of the inlet high-pressure port, both flow rate and power will reduce. You can check all other performance parameters in short, normal and complete thermodynamic reports which can be viewed from the Top Menu > View > Reports > Thermodynamic > Short/ Normal/ Complete.

3 Oil injected ORC expander

To evaluate performance of oil the injected screw expander used in Organic Rankine Cycle, please Save As this case under the name SCORG_35_Expander_Refrigeration Tutorial.

In tab Design Exploration click with the right button to any of Design points and select option “Delete all Design points”. Also de-select Vlume Index, GAPI and GAPR in the relevant inputs.

In Profile Setup inputs select Profile Choice to: Demonstrator profile and change the value Z1 to 4. In Profile Elements Inputs change R to 14.75, R0 to1, R2 to 1, R3 to 5 and R4 to 1, as shown below

Profile Setup

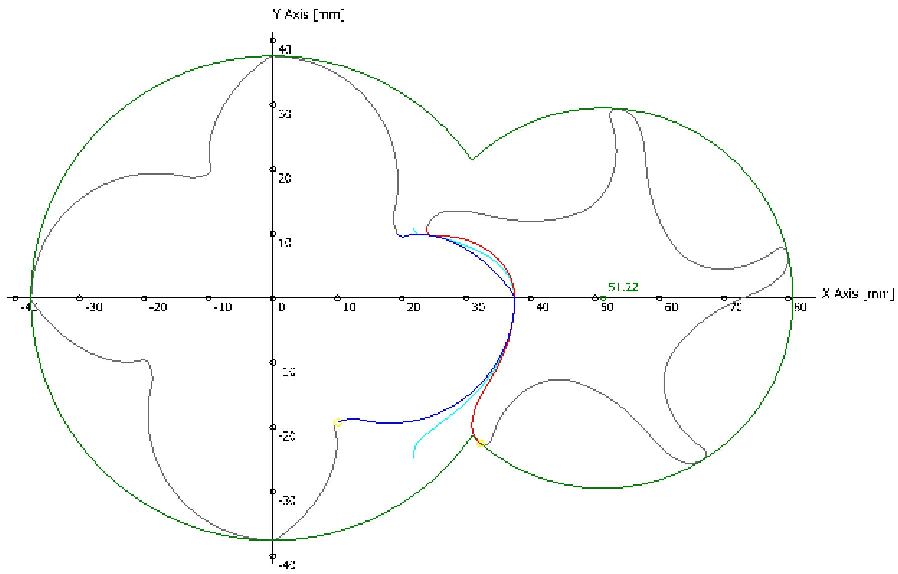
Profile Choice	Demons...		
Axis Distance	51.223		mm
Z1	4		
Z2	5		
GAPI	0.05	☐	mm
GAPR	0.05	☐	mm
GAPA	0.08	☐	mm

Profile Elements

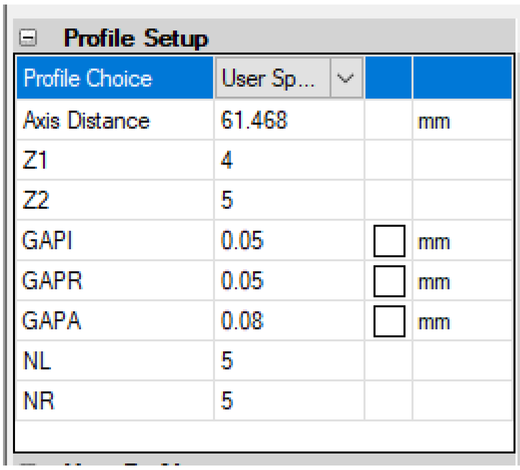
R	14.75	mm
R0	1	mm
Excentricity	0	mm
Tooth Tip Angle	0	Deg
R1	0	mm
R2	1	mm
R3	5	mm
R4	1	mm
α1	17.189	Deg
α2	17.189	Deg
Exponent	0.5	
Relative point spacing	0.031	
Clearance Distribution	Clearences	

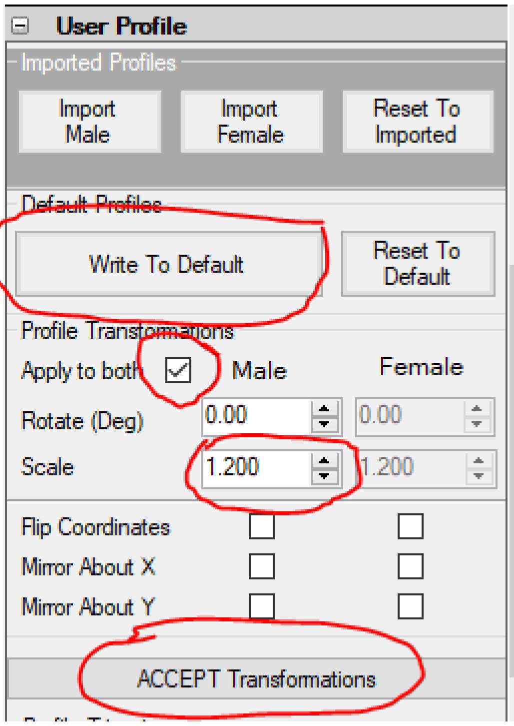
Generate Profile

Click on Generate Profile button below Profile Elements Inputs. This should generate the Demonstrator profile with 4/5 lobes as shown in the figure below

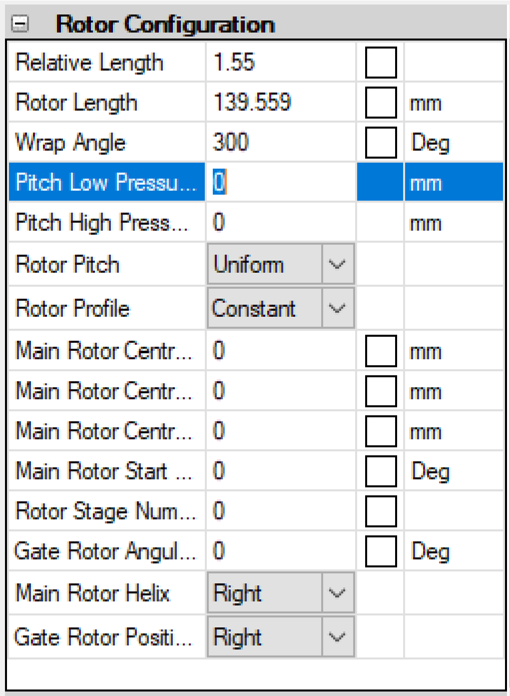


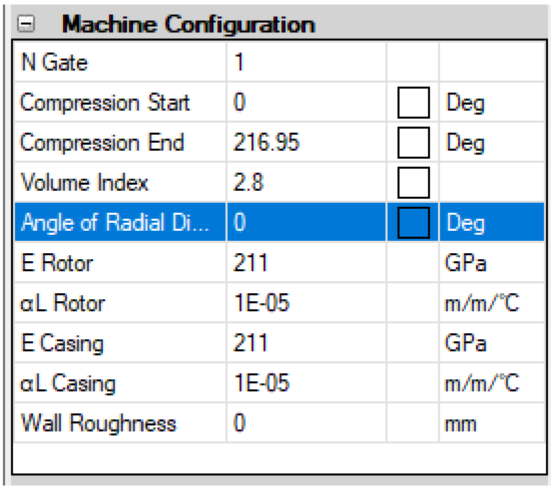
In the Profile setup change Profile Choice to: User Specified Profile. Then In user Profile Inputs select "Apply to both" and increase the scale factor to 1.2. Accept Transformation and Write to Default.





In Rotor Configuration Inputs set the Relative length to 1.55 and Wrap angle to 300 Deg. In Machine Configuration Inputs set Volume Index to 2.8.





This should now complete setting of 4/5 Expander with 90.038 mm main rotor ready for calculation of this machine in a ORC system. In Working Fluid Inputs switch Fluid to Real Gas, open Form NIST and select R245FA from the list of fluids.

In Working Conditions Inputs set Wtip to 40, Tevap to 20 degC, Tcond to 80 degC and Tr to 85 degC.

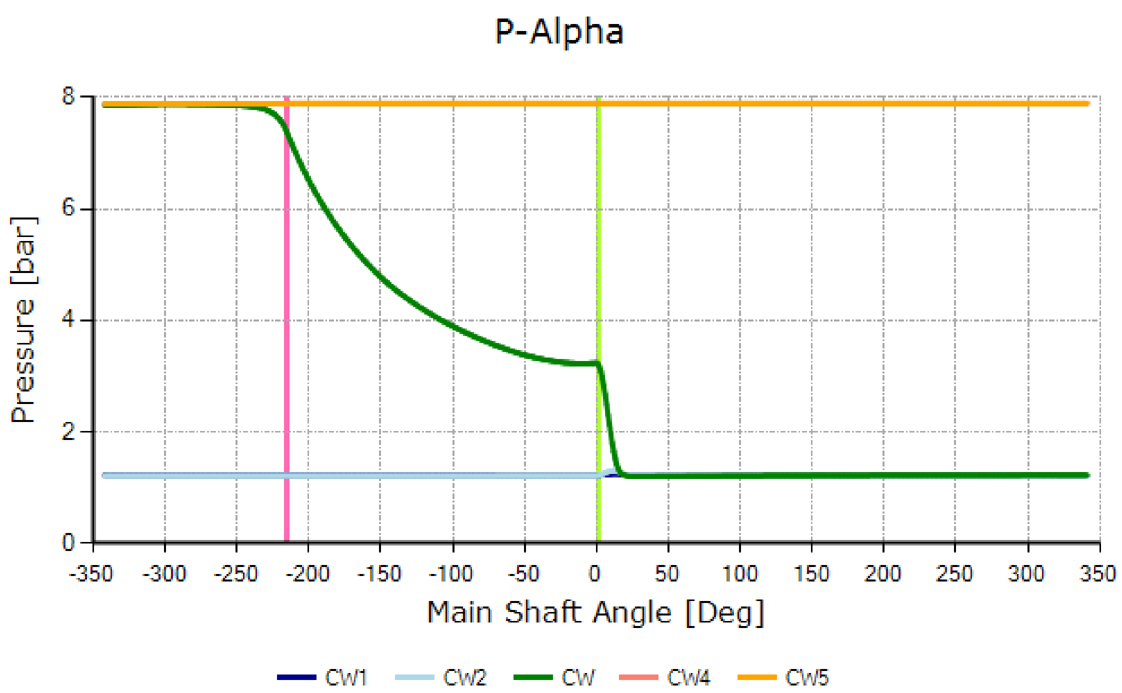
Working Fluid

Fluid	Real Gas	
Fluid name	R245FA	
Number of components	1	
Tc	153.86	℃
Form NIST	Form NIST...	

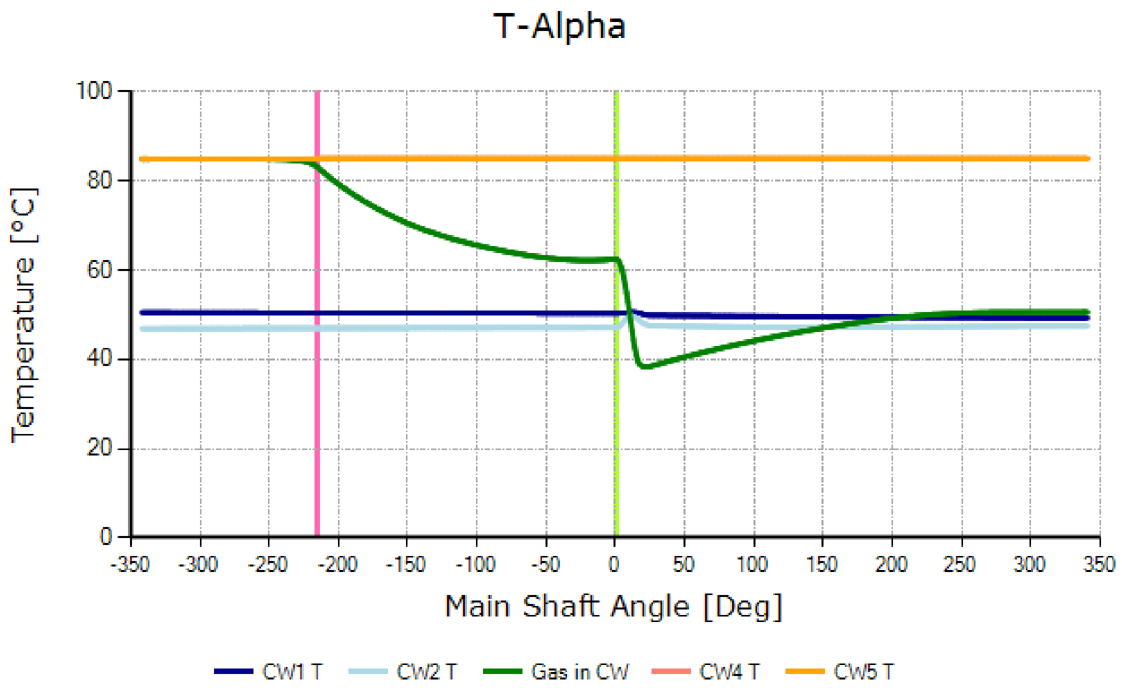
Working Conditions

Wtip	40	m/s
Rotor Speed	8484.7	RPM
P0	1.231	bar
Pr	7.89	bar
T0	20	℃
Tr	85	℃
Tevp	20	℃
Tcond	80	℃
T Ambient	19.85	℃
Include heat transfer	No	
X	1	

The resulting cycle pressure is shown in the diagram below.



Corresponding cycle temperature is shown in the diagram below and the detailed performance is shown in the following snapshot of the Normal thermodynamic results.

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SCORG - Thermodynamic Performance Calculation

          Date: 18/01/2022 21:39:36


Gas properties    -   Real gas  (REFPROP 10)
     Critical parameters
     component#  name        T(K)        P(kPa)      rho(mol/K)  x (kg/kg)
     1           R245FA      427.01      3651.000    3.875       1.00000

Machine: Expander
     Lobe combination  : 4/5
     Size              : 90/155 28
     Mechanical seals  : 1

==============================================

T1    = 50.62 degC     T2    = 85.01 degC
P1    = 1.231 bar      P2    = 7.89  bar
Moil  = 0     kg/s     Toil  = 40.01 degC
                       Poil  = -1    bar

Volume Index Vi        = 2.8
Pressure Ratio Pi      = 3
Speed                  = 8484.7 rpm
Tip speed              = 40     m/s

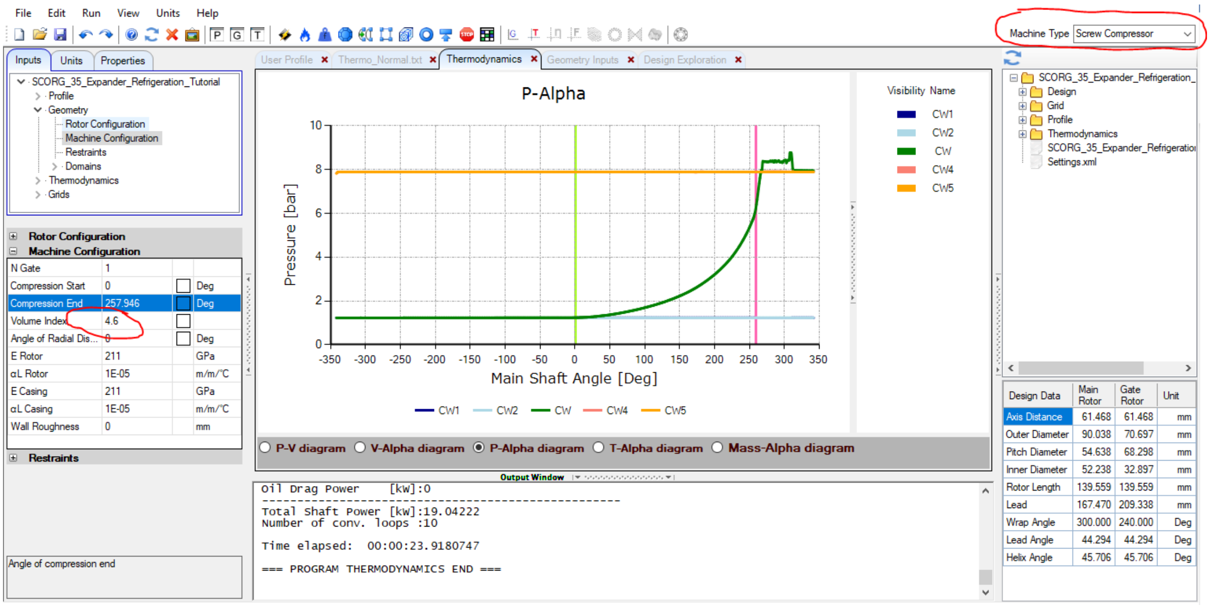
Volume flow rate       = 9.96    m3/min
                       = 597.6   m3/h
Mass flow rate         = 3784.8  kg/h
                       = 1.05    kg/s
Volumetric efficiency  = 94.39   %

Power (excl. gearbox)  = -32.12  kW
                       = -43.07  HP
Specific power         = 3.23    kW/m3/min
Adiabatic efficiency   = 79.68   %

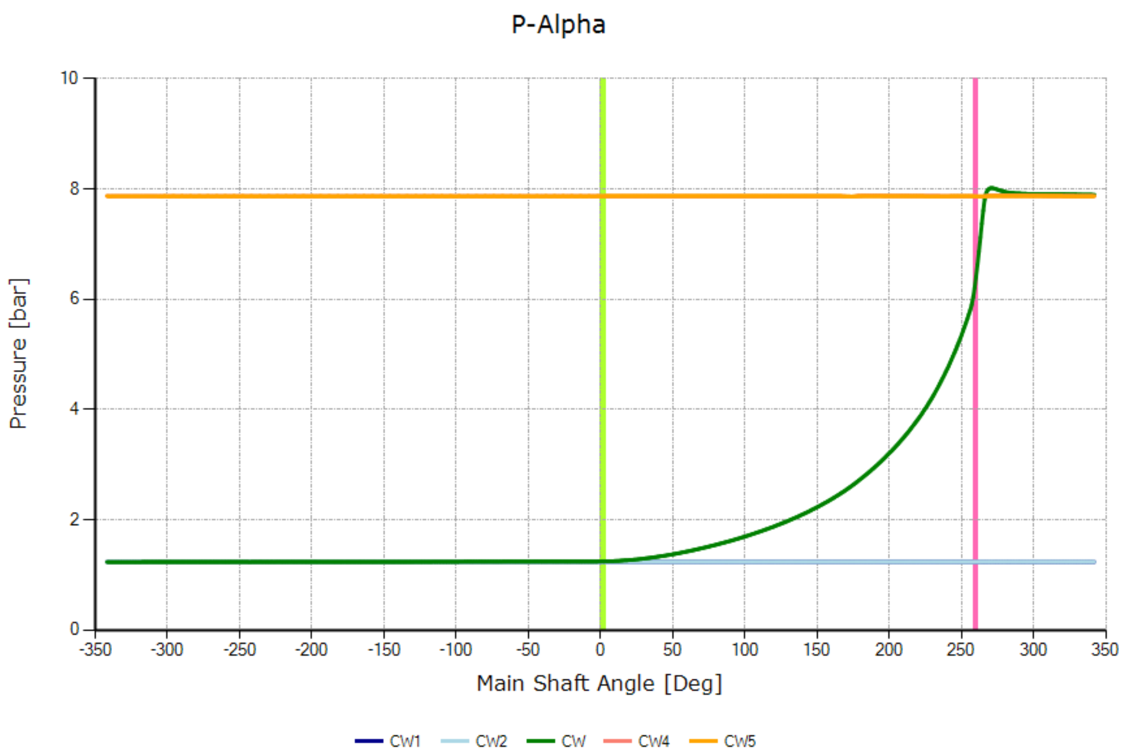
Theoretical mass flow  = 4009.88 kg/h
Discharge mass flow    = 3784.8  kg/h
```

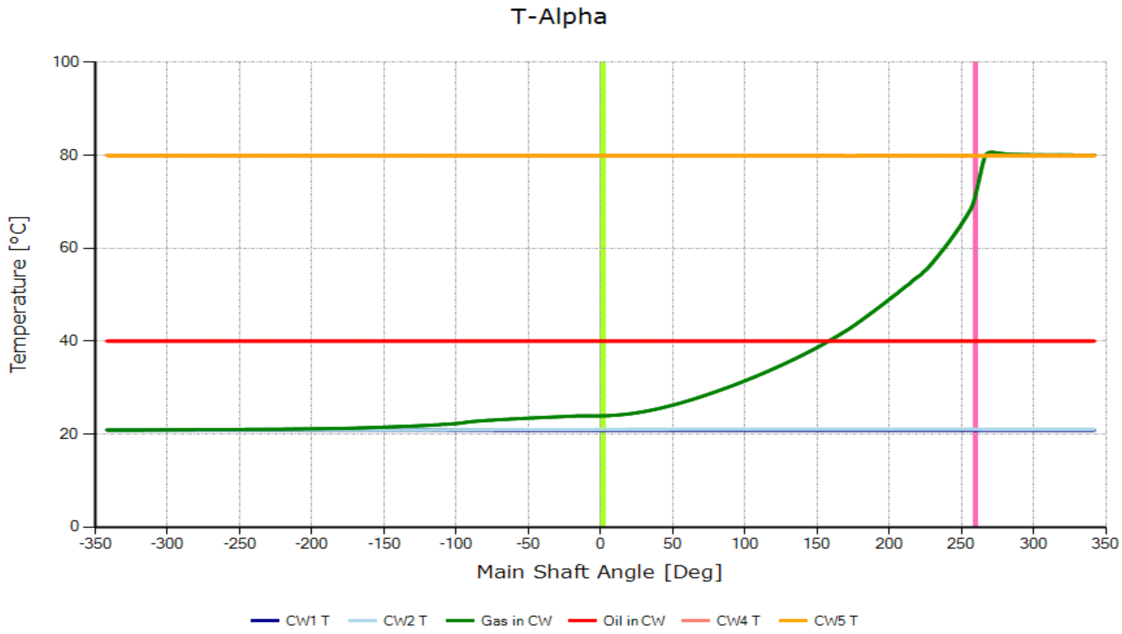
4 Calculate refrigeration compressor

To calculate the same machine as screw compressor at the same conditions, simply set the Machine Type top Screw Compressor. Change Vi to 4.6.



The results of performance predictions calculation is shown in diagrams and Normal report below




T-Alpha
Temperature [°C]
Main Shaft Angle [Deg]
100
80
60
40
20
0
-350
-300
-250
-200
-150
-100
-50
0
50
100
150
200
250
300
350
CW1 T
CW2 T
Gas in CW
Oil in CW
CW4 T
CW5 T

```
SCORG - Thermodynamic Performance Calculation


          Date: 18/01/2022 21:47:02



Gas properties    -   Real gas  (REFPROP 10)
     Critical parameters
     component#  name        T(K)        P(kPa)      rho(mol/K)  x (kg/kg)
     1           R245FA      427.01      3651.000    3.875       1.00000

Machine: Oil Free Compressor
     Lobe combination  : 4/5
     Size              : 90/155 46
     Mechanical seals  : 1

=====================================================

Tevap = 20.01 degC           Tcond = 80.01 degC
T1    = 20.02 degC           T2    = 80.62 degC
P1    = 1.231 bar            P2    = 7.89  bar
Moil  = 0     kg/s           Toil  = 40.01 degC
                             Poil  = -1    bar

Volume Index Vi              = 4.6
Pressure Ratio Pi            = 5.11
Speed                        = 8484.7 rpm
Tip speed                    = 40     m/s

Volume flow rate             = 3.85    m3/min
                             = 231     m3/h
Mass flow rate               = 1643.97 kg/h
                             = 0.46    kg/s
Volumetric efficiency        = 87.39   %

Power (excl. gearbox)        = 19.04   kW
                             = 25.53   HP
Specific power               = 4.94    kW/m3/min
Adiabatic efficiency         = 81.89   %

Theoretical mass flow        = 1881.18 kg/h
Discharge mass flow          = 1643.97 kg/h

Refrigeration capacity       = 50.99   kW
Coefficient of performance   = 2.76

Heat pump capacity           = 70.58   kW
Coefficient of performance   = 3.82
```

5 Summary

This document describes the steps to setup and calculate performance of two screw expanders, one for expansion of compressed air and another for use in Organic Rankine Cycle with refrigerants. More detailed information on using SCORG can be found in user guide (SCORG, 2022). Thermodynamic calculations are used as the preliminary performance predictions which could be utilised for design of screw machines, initial conditions for CFD and FEM.

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End of Document

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