# Development of a semi-analytical model of volumetric expander for system-level simulation.

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**Abstract:**

Organic Rankine cycles are particularly well suited for recovering energy from low-grade heat sources, such as industrial waste, engine exhaust gas or solar concentrated power. In low-capacity systems, volumetric expanders are often preferred to turbomachines because of their reliability, robustness, low rotational speed and their ability to handle high pressure ratios… Different types of machines have been investigated and successfully tested by the authors and tools have been developed in order to analyse experimental data. Semi-empirical model was built to analyse losses, detect potential improvement and simulate performances. This paper present a simple and fast-computing semi-analytical model useful for simulate dynamic system integrating volumetric expander. This model is validated on experimental data and compare to black-box model.

**Keywords:**

ORC, Expander, Model

# 1 Introduction

In the actual energy context, rational use of energy became a world major issue. Among different technologies, organic Rankine cycle (ORC) systems are more and more envisaged as a solution for small-scale power generation in applications valorising the following heat sources: waste heat recovery, geothermal heat or solar thermal energy. For low capacity ORC, volumetric expanders are well suited and often preferred to turbo-machines.

In order to investigate volumetric expanders and ORC system, the authors developed tools to assist experimental, modelling and simulation efforts. Until now, several experimental campaigns have been performed [1-6]. In order to facilitate analysis and assessment of experimental results, GPEexp tools was developed [7]. This tools allowed to asses quality of experimental data, to detect outliers and can help to understand which input variable are most relevant [8]. Once experimental results are obtained and assessed, model can be developed in order better understand the different sources of losses, to detect potential improvement and to simulate the performances. In this context, semi-empirical models was developed and successfully calibrated and exploited [1] [6]. Finally expanders have to be simulated at the ORC system level and in a dynamic behaviour. For this purpose, faster and simpler models have to be developed. This paper proposes such models based on analytical physically-based expressions denoted "semi-analytical model".

First, the semi-analytical model is described. Then it is applied to piston and scroll expanders. Finally, the model is compared to similar models.

# 2 Semi analytical model

The proposed model is based on analytical expressions derived by simplification of the real process. The simplification consists in considering theoretical processes and treats fluid as ideal gases. Then, several parameters of the analytical expression are fitted in order that solutions of the equations best match the data given by a more sophisticated and calibrated model or experimental data.

## 2.1 Theoretical process

The theoretical expansion process into a volumetric expander considered for the model is illustrated in Fig. 1. This process is divided in seven theoretical steps:

- Isenthalpic supply pressure drop ($\Delta P_{su}$) from $P_{su}$ to intake pressure $P_{in} = P_1 = P_2$
- 1-2: isobaric intake
- 2-3: isentropic expansion
- 3-4: constant machine volume expansion
- 4-5: isobaric exhaust
- 5-6: isentropic compression
- 6-1: constant machine volume compression

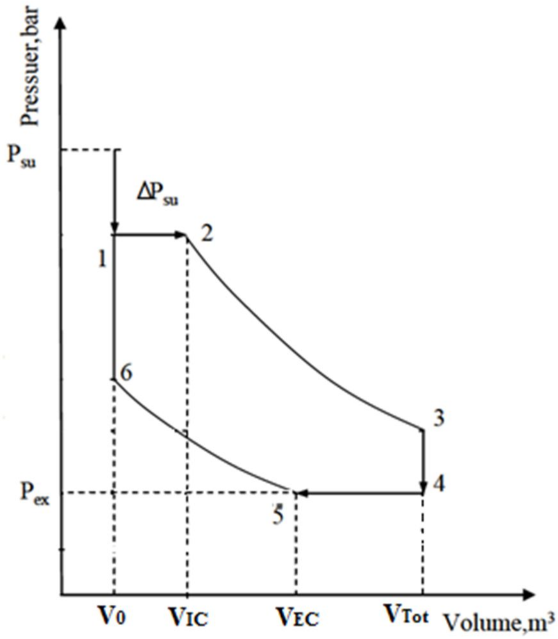


*Fig. 1: Theoretical process of the expansion into a volumetric expander.*

## 2.2 Indicated work

The indicated work provide by the working fluid is given by:

$$W_{in} = P_1.(V_2 - V_0) + \frac{V_2}{v_2}.(u_2 - u_3) - P_4.(V_{Tot} - V_5) - \frac{V_5}{v_5}.(u_6 - u_5) \quad (1)$$

which is equivalent to:

$$W_{in} = \frac{V_2}{v_2}.(h_2 - h_3) + V_{Tot}.(P_3 - P_4) - \frac{V_5}{v_5}.(h_6 - h_5) - V_0.(P_1 - P_6) \quad (2)$$

Considering the hypothesis of ideal gases, (2) becomes:

$$W_{in} = \frac{P_2.V_2}{r.T_2}.cp.(T_2 - T_3) + V_{Tot}.(P_3 - P_4) - \frac{P_5.V_5}{r.T_5}.cp.(T_6 - T_5) - V_0.(P_1 - P_6) \quad (3)$$

Introducing the following geometrical ratios:

$$rv_e = \frac{V_{Tot}}{V_{IC}} = \frac{1}{CO} \ , \ rv_c = \frac{V_{EC}}{V_0} \ , \ CO_c = \frac{V_{EC}}{V_{Tot}} \ , \ \mu = \frac{V_0}{V_{Tot}} \quad (4)$$

often denoted as expansion built-in volume ratio, recompression built-in volume ratio, exhaust cut-off and clearance volume ratio respectively, (4) can be written as:

$$W_{in} = P_{in}.V_{Tot}.\left[\frac{1}{rv_e.k}\left(1 - rv_e^{1-\gamma}\right) - \frac{CO_c}{r_p.k}.\left(rv_c^{\gamma-1} - 1\right) + rv_e^{-\gamma} - \frac{1}{r_p} + \mu\left(\frac{rv_c^{\gamma}}{r_p} - 1\right)\right] \quad (5)$$

where $\gamma$ is the isentropic ratio, $k = \frac{\gamma-1}{\gamma}$ and $P_{in} = P_1 = P_2$ is the intake pressure.

## 2.3 Shaft power

Knowing the indicated work, the indicated power is given by:

$$\dot{W}_{in} = W_{in}.N_{rot} \tag{6}$$

where $N_{rot}$ is the rotational speed of the expander.

The shaft power is the indicated power diminished by the mechanical losses:

$$\dot{W}_{sh} = \dot{W}_{in} - \dot{W}_{loss} \tag{7}$$

As proposed in [6] the mechanical losses are assumed to be a function of the indicated power and rotational speed:

$$\dot{W}_{loss} = a.\dot{W}_{in} + b.RPM^2 \tag{8}$$

## 2.4 Mass flow

The effective mass flow rate is the sum of the internal and the leakage mass flow rate.

$$\dot{M} = \dot{M}_{in} + \dot{M}_{leak} \tag{9}$$

Difference between the mass in the cylinder when the inlet valve closes and opens multiplied by rotational speed give the internal mass flow rate.

$$\dot{M}_{in} = (m_2 - m_6).N_{rot} \tag{10}$$

Considering ideal gases, (10) can be written as:

$$\dot{M} = \left(\frac{P_2.V_2}{r.T_2} - \frac{P_6.V_6}{r.T_6}\right).N_{rot} \tag{11}$$

Assuming an isenthalpic pressure drop and an ideal gas, temperature in state 2 is equal to the supply temperature $T_{su}$. For temperature in state 6, a fully isentropic expansion is considered to compute temperature at point 5. Knowing temperature at point 5, temperature at point 6 can be computed:

$$T_6 = T_5.rv_c^{\gamma-1} = T_2.rp^{\frac{1-\gamma}{\gamma}}.rv_c^{\gamma-1} = T_{su}.rp^{\frac{1-\gamma}{\gamma}}.rv_c^{\gamma-1} \tag{12}$$

Finally, the internal mass flow rate is given by:

$$\dot{M}_{in} = \left[P_{in}.V_{IC} - P_{ex}.V_{EC}.rp^{\frac{\gamma-1}{\gamma}}\right].\frac{N_{rot}}{r.T_{su}} \tag{13}$$

Leakage flow is computed as chocked isentropic flow through a fictive nozzle of cross sectional area $A_{leak}$ between supply and exhaust. For ideal gases, this type of flow is describe by:

$$\dot{M}_{leak} = A_{leak}.\sqrt{\frac{2.P_{su}^2}{r.T_{su}}.\frac{\gamma}{\gamma+1}}.\left(\frac{2}{\gamma+1}\right)^{\frac{1}{\gamma-1}} \tag{14}$$

## 2.5 Pressure drop

Equation (5) and (13) depend on $P_{in}$ which depends on the supply pressure drop. As for leakage flow, this pressure drop is computed as the fluid pass through a fictive nozzle of cross sectional area $A_{su}$ but her, the flow is considered as subsonic. Then, the mass flow through the supply nozzle is:

$$\dot{M} = A_{su}.\frac{P_{thr}}{r.T_{thr}}.\sqrt{2.cp.T_{su}.(1 - r_{p,su}^{\frac{1-\gamma}{\gamma}})} \quad (15)$$

where the subscript $thr$ design the state of the fluid at the throat of the nozzle and $r_{p,su} = \frac{P_{su}}{P_{in}}$.

In order to find an analytical and explicit expression of $r_{p,su}$, the leakage flow is neglected and pressure ratio in (13) is considered as total pressure ratio $r_{p,tot} = \frac{P_{su}}{P_{ex}}$. Then, (15) and (13) can be combined to give:

$$rp_{su} = \left(1 - \frac{\left[V_{IC} - V_{EC}.r_{p,tot}^{\frac{-1}{\gamma}}\right]^2 .\left(\frac{N_{rot}}{A_{su}}\right)^2}{2.cp.T_{su}}\right)^{\frac{\gamma}{(1-\gamma)}} \quad (16)$$

## 2.6 Global model, parameters and fitting

To recap, the model is able to compute the mass flow rate and the shaft power of the expander in terms of supply pressure, exhaust pressure, supply temperature and rotational speed.

Mass flow rate is computed combining (16), (9), and (14) and depends on:

- two built-in geometrical parameters, $V_{IC}$ and $V_{EC}$,
- two fictive areas, $A_{su}$and $A_{leak}$
- isentropic expansion ratio $\gamma$

In order to have better match when fitting the model, different isentropic expansion ratios and supply areas will be considered. Thereafter the $\gamma$ and $A_{su}$ used to compute the mass flow rate will be denoted as $\gamma_m$ and $A_{su,m}$

In the same manner, shaft power is computed combining (16), (5), (6), (7) and (8) and depends on:

- two additional built-in geometrical parameters, $V_{tot}$ and $V_0$,
- one fictive area denoted $A_{su,w}$ used in (16) (the $\gamma$ used in (16) to compute power is $\gamma_m$)
- two isentropic expansion ratios, $\gamma_e$ and $\gamma_c$, respectively for expansion and compression (so related to $rv_e$ and $rv_c$ $in$ (5))
- two parameters related to the mechanical losses, $a$ and $b$ in (8)

To fit this nonlinear model, the Matlab function "NonLinearModel.fit" is used.

# 3 Example of fitting

The semi-analytical model presented hereinabove is now tested on two experimental data sets in order to check its ability to predict volumetric expander characteristics. The first experimental results are associated to a piston expander and are described in [6]. The second setoff experimental data is related to a scroll expander tested in [5].

## 3.1 Piston expander

The results of the fitting process are plots in Fig. 2 and are compared to results of the semi-empirical model described in [6]. The fitting process of the semi-analytical model gives coefficients of determination of $R^2$=98.5 % and $R^2$=94.7 % for the mechanical power and mass flow rate respectively. It can be seen that the semi-analytical model gives good results comparable to those given by the semi-empirical model. For these results, built-in geometrical parameters are the actual values of the tested expander. Other parameters are listed in Table 1.

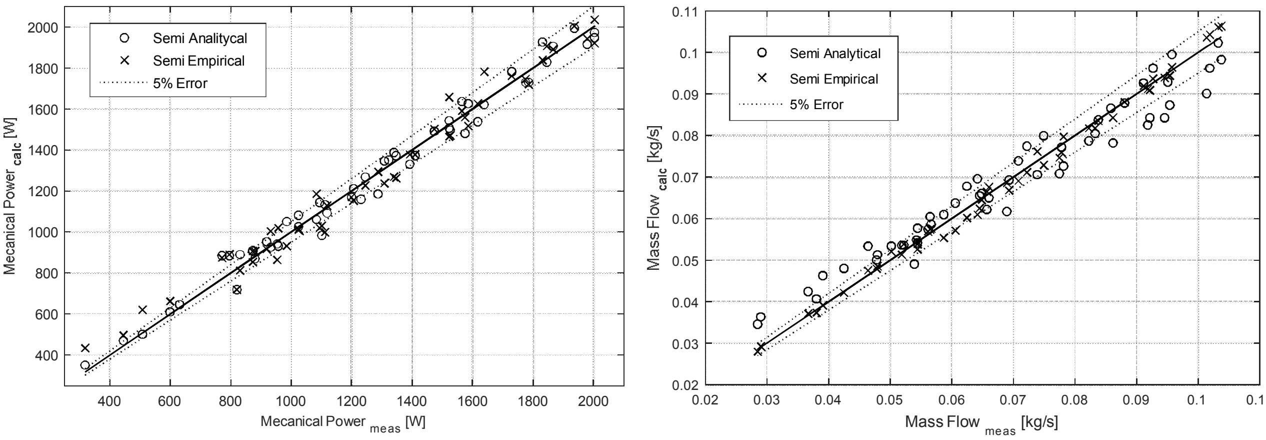


*Fig. 2. Calculated versus measured values of the semi analytical and the semi empirical models for mechanical power (left) and mass flow rate (right) of piston expander.*

*Table 1. Fitted parameters of the semi analytical model for piston expander.*

| $\gamma_m$[-] | $A_{su,m}$ [m²] | $A_{leak}$ [m] | $\gamma_e$ [−] | $\gamma_c$ [−] | $A_{su,w}$ [m²] | a [-] | b [W.min²] |
|---|---|---|---|---|---|---|---|
| 1.04 | 3.06 x $10^{-6}$ | 4 x $10^{-7}$ | 0.92 | 0.5 | 1.79 x $10^{-6}$ | 0.16 | 8.2 x $10^{-6}$ |

## 3.2 Scroll expander

The results of the fitting process are plotted in Fig. 3. The semi-analytical model gives coefficients of determination of $R^2$=98.1% and $R^2$=83.9% for mechanical power and mass flow rate respectively. The model for mechanical power shows good fitness with measurements while mass flow shows deviation for low and high mass flow. This deviation for the mass flow rate can eventually be adjusted using a variable leakage area as suggested in [9].

As for piston expanders, built-in geometrical parameters are the actual values. It has to be noticed that for scroll expanders (as for other expanders without clearance and recompression such as screw expander) $V_0 = V_{EC} = 0$, simplifying (5) (13) and (16) and making $\gamma_c$ useless. Results for other parameters are listed in Table 2. The fitting process gives initial value and value order of $10^7$ for $A_{su,m}$ and $A_{su,w}$ respectively, showing that no pressure supply drop have to be applied.

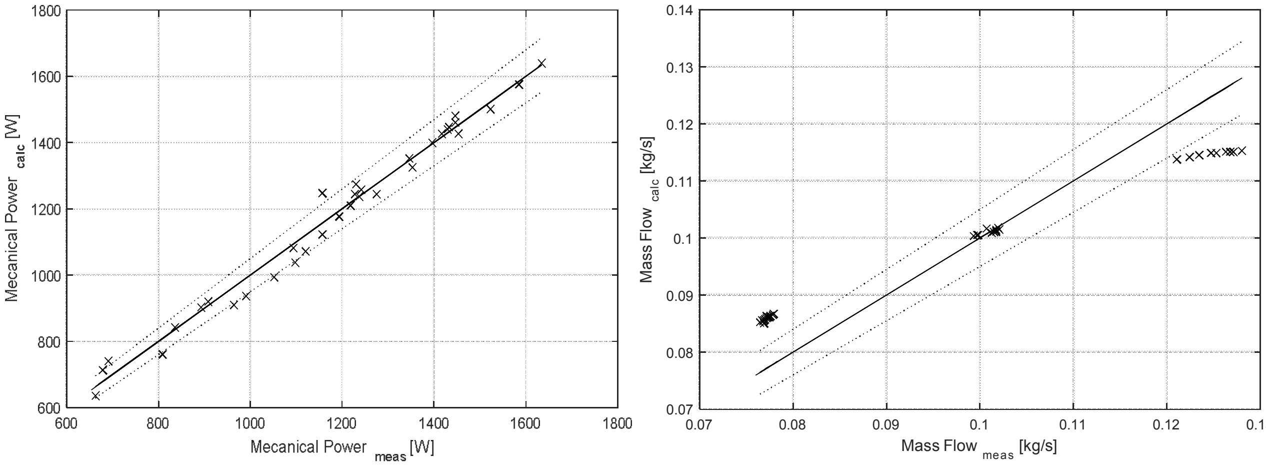


*Fig. 3. Calculated versus measured values of the semi analytical model for mechanical power (left) and mass flow rate (right) of scroll expander.*

*Table 2. Fitted parameters of the semi analytical model for scroll expander.*

| $\gamma_m$[-] | $A_{su,m}$ [m²] | $A_{leak}$ [m] | $\gamma_e$ [−] | $A_{su,w}$ [m²] | a [-] | b [W.min²] |
|---|---|---|---|---|---|---|
| 1.14 | / | 2.54 x $10^{-6}$ | 1.22 | / | 0.315 | 7.65 x $10^{-7}$ |

# 4 Comparison with black-box model

The semi analytical model proposed in this work can be compared to black-box models such as the model based on Pacejka's equation used in [3] or second-order polynomial correlation models used in [9]. Indeed, all these models are based on simple analytical expressions allowing fast and simple calibration and implementation. The difference is that the semi analytical model proposed in this paper has a physical meaning.

The physical meaning of the proposed model allows for a better extrapolation of results (beyond the range of data used for calibration) than black-box models. In order to evaluate the ability of extrapolation of these three different models, the 60 measured points of [6] used in section 3.1 are divided into two sets, a "fit set", used to calibrate the model and a "extrapolation set" used to test the extrapolation capability of the model.

In this example the fit set is composed of 29 points with supply pressure of 18 and 21 bar and the extrapolation set is made of the 31 remaining points with supply pressure of 24, 27 and 30 bar. The results can be observed in Fig. 4 and coefficients of determination for the fit set and for the whole set are listed in Table 3. It can be seen that the three models well fit the experimental results for the fit set. When keeping the parameters found with the fit set and applying the model on the whole set, the polynomial model is no more capable of simulate the mass flow and the mechanical power with $R^2$ becoming -294.8% and -159.9% respectively. The model based on Pacejka's model show ability to extrapolate the mass flow rate but not the power, while the semi-analytical model keeps $R^2$ upper than 90% for the mass flow rate and 97% for the mechanical power.

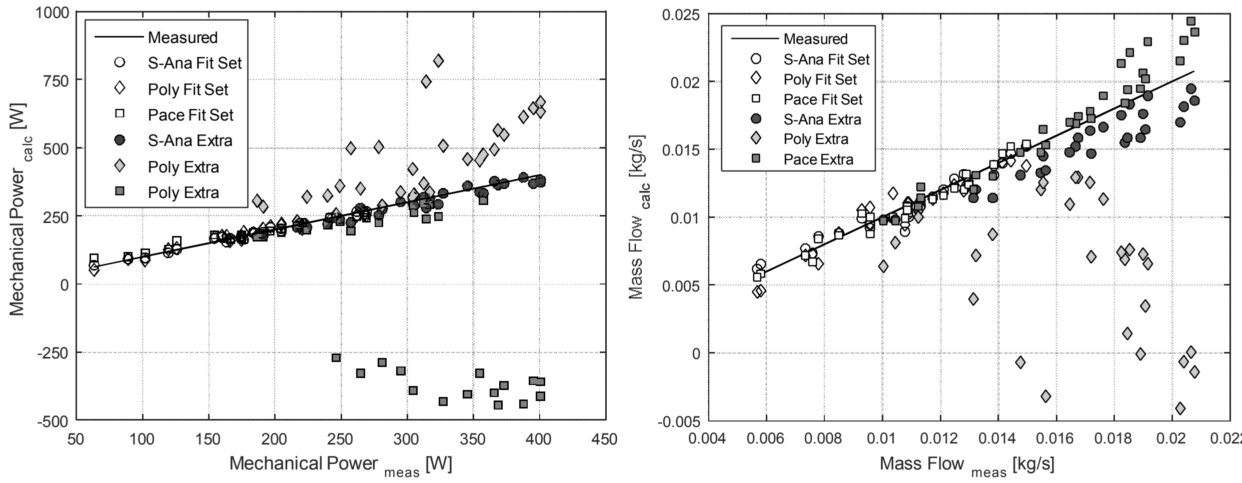


*Fig. 4. Comparison of the mechanical power (left) and mass flow rate (right) extrapolation ability for tree different models (Semi Analytical, Polynomial and Pacejka's).*

*Table 3. Coefficients of determinations on the fit set and on the whole set.*

| **$R^2$ [%]** | Semi Analytical | $2^{nd}$order Polynomial | Pacejka's |
|---|---|---|---|
| Fit Set, Mass Flow | 95.4 | 92.1 | 96.5 |
| Whole set, Mass Flow | 90.8 | -294.8 | 92.3 |
| Fit Set, Mechanical Power | 98.3 | 95.4 | 92.1 |
| Whole set, Mechanical Power | 97.3 | -159.9 | -1247.9 |

# 5 Conclusion

In order to easily simulate volumetric expanders integrated into ORC systems, a simple and fast computing semi-analytical model has been developed and assessed. This model is able to predict, with a good agreement, performances of different types of volumetric expanders. Moreover, this model has a certain ability to extrapolate results, which is note the case of other simple and fast computing black-box models.

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# References


[1] Lemort V, Quoilin S, Cuevas C, Lebrun J. Testing and modeling a scroll expander integrated into an Organic Rankine Cycle. Appl Therm Eng. 2009 Oct;29(14-15):3094–102.

[2] Lemort V, Declaye S, Quoilin S. Experimental characterization of a hermetic scroll expander for use in a micro-scale Rankine cycle. Proc Inst Mech Eng Part J Power Energy. 2012 Feb 1;226(1):126–36.

[3] Declaye S, Quoilin S, Guillaume L, Lemort V. Experimental study on an open-drive scroll expander integrated into an ORC (Organic Rankine Cycle) system with R245fa as working fluid. Energy. 2013 juin;55:173–83.

[4] Dumont O, Quoilin S, Lemort V. Experimental investigation of a reversible heat pump/organic Rankine cycle unit designed to be coupled with a passive house to get a Net Zero Energy Building. Int J Refrig. 2015 Jun;54:190–203.

[5] Dickes R, Dumont O, Declaye S, Quoilin S, Bell I, Lemort V. Experimental investigation of an ORC system for a micro-solar power plant. In Purdure, USA; 2014.

[6] Oudkerk JF, Dickes R, Dumont O, Lemort V. Experimental performance of a piston expander in a small- scale organic Rankine cycle. IOP Conf Ser Mater Sci Eng. 2015;90(1):012066.

[7] squoilin/GPExp [Internet]. GitHub. [cited 2016 Feb 11]. Available from: https://github.com/squoilin/GPExp

[8] Quoilin S, Schrouff J. Assessing the Quality of Experimental Data with Gaussian Processes: Example with an Injection Scroll Compressor. 2014 [cited 2015 Dec 28]; Available from: http://docs.lib.purdue.edu/icec/2377

[9] Dickes R, Dumont O, Legros A, Quoilin S, Lemort V. Analysis and comparison of different modeling approaches for the simulation of a micros-scale organic Ranking cycle power plant. In Brussel, Belgium; 2015.