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Extrapolability and limitations of a semi-empirical model for the simulation of volumetric expanders

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Abstract

Many different modelling approaches can be used to simulate the performance of expansion devices in ORC power systems. A decade ago, researchers proposed a semi-empirical modelling method that can be used to generally characterize volumetric expanders (e.g. scroll, screw, piston or vane machines). The modelling approach relies on a limited number of physically meaningful equations which decompose the expansion process into a number of consecutive steps. Besides of under- and over-expansion losses (due to the fixed built-in volumetric ratio of the machine), the model can account for pressure drops at the inlet and outlet ports, internal leakages, mechanical losses, recompression effects and heat losses to the environment. The semi-empirical model relies on different parameters that must be properly tuned according to experimental (or manufacturer) data. In practice, the reference database used for the parameters calibration (e.g. the measurements gathered on a test rig) does not necessarily cover the entire range of conditions onto which the model will be evaluated. The capability of the semi-empirical model to behave well in extrapolated conditions must therefore be assessed. In this work, a detailed analysis of the extrapolation performance of this semi-empirical model is conducted. More specifically, the semi-empirical model behavior is analyzed after being calibrated with different ranges of reference conditions. A study of the smallest reference dataset to ensure a decent modelling accuracy is proposed. Finally, the influence of the parameters guess values and the optimization algorithm on the model calibration is assessed.

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Keywords: Volumetric expander, semi-empirical model, grey-box model, extrapolability, limitations

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1. Introduction

This paper is dedicated to the analysis of a semi-empirical model for the simulation of volumetric expanders. After a brief description of the concept of *semi-empirical* modelling and the expander model itself (section 1), the paper proposes a methodology to assess the extrapolation capability of such model when evaluated out of its calibration

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domain (section 2). In section 3, results from an experimental case study are analyzed to discuss the effects of the calibration range and the influence of the initial guesses. Finally, guidelines are proposed to ensure a reliable parameters calibration and a proper use of such expander semi-empirical model (section 4).

Nomenclature			**Subscript**	
A	Area	(m^2)	amb	Ambient
d	Diameter	(m)	ex	Exhaust
err	Error	(-)	leak	Leakage
MAE	Mean Average Error		meas	Measured
$\dot{m}$	Mass flow rate	(kg/s)	pred	Predicted
N	Number of points	(-)	sh	Shaft
U	Heat transfer coefficient	(W/(m.K))	su	Supply
C	proportional mechanical loss	(-)	0	Clearance
RMSE	root mean square error	(-)		
T	Temperature	(°C)		
V	Volume	(m^3)		
$\dot{W}$	Power	(W)		
y	Output			
α	Constant mechanical loss	(-)		

1.1. Notion of semi-empirical modelling

Components in a thermal system can be simulated following various modelling approaches which could be classified in three groups: black-box (*empirical*) models, grey-box (*semi-empirical*) models and white-box (*deterministic*) models. Black-box models are referring to empirical modelling methods which do not describe the physics of the processes. In the case of an expander, for example, such models would characterize the machine performance through its isentropic and volumetric efficiencies by means of constant empirical values or polynomial regressions. Although fast to implement, to calibrate and to simulate, black-box models do not ensure reliable predictions in extrapolated conditions [1]. On the other hand, white-box models implement equations describing all the physical and the chemical phenomena in the system. Although more accurate, deterministic models are often computational intensive and, consequently, too slow for system-level simulations. Examples of deterministic models for volumetric expanders can be found in [2,3]. Semi-empirical models are a compromise between the two aforementioned methods. They rely on a limited number of physically meaningful equations which describe the most influent phenomena in the system. They offer a good trade-off between simulation speed, calibration efforts, modelling accuracy and extrapolation capabilities. Semi-empirical models have extensively been used for the sizing and the modelling of heat exchangers, compressors, expanders and pumps [4-9].

1.2. *Semi-empirical model of volumetric expanders*

In this work, the semi-empirical model investigated to simulate volumetric expanders is an extended extended version of the model proposed by Lemort et al. [6]. One advantage of this approach is its common framework to simulate different types of technologies (scroll, screw, piston, vane…) [9]. Besides of under- and over-expansion losses (due to the fixed built-in volumetric ratio of the machine), the model can account for pressure drops and heat transfers at the inlet and outlet ports of the machine, internal leakages, mechanical losses, heat losses to the environment and recompression phenomena. Depending on the case study, the level of details of the model may be adjusted by adding or removing some parameters. As depicted in Fig. 1, the expansion process of the fluid is divided into successive steps i.e. a supply pressure drop (su ➔ su_1), a supply heat transfer (su_1 ➔ su_2), a two-stage expansion (su_2 ➔ ex_2), an exhaust heat transfer (ex_3 ➔ ex_2), an exhaust pressure drop (ex_2 ➔ ex_1), an internal leakages flow

(su_2 ➔ ex_1 in black) and a recompression flow (ex_1➔su_2 in green). The supply and exhaust pressure drops are modelled as an isentropic flow through a converging nozzles, whose diameters d_{su} and d_{ex} respectively, are parameters to be identified. The three heat transfer (supply, exhaust and ambient) are characterized with nominal heat transfer coefficients i.e. $AU_{su,nom}$, $AU_{ex,nom}$ and AU_{amb}.

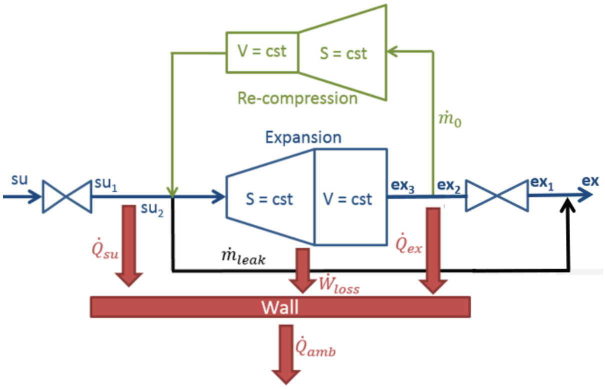

Fig. 1. Schematic representation of the overall expander model (the green part – re-compression- is only used in the case of the piston expander)

Leakages are lumped into one parameter as an isentropic flow through a simply convergent nozzle whose diameter, d_{leak}, is another parameter to identify. Mechanical losses are computed with a constant term (α) and a loss proportional to the rotational speed (by means of a losses torque C_{loss}). Finally, in the case of piston expanders, the recompression losses due to the fluid trapped inside the clearance volume (V_0) is modelled by means of two-stage compression as proposed by [10]. For further information regarding the governing equations of this model, refer to [6].

Ultimately, the modelling of most volumetric expanders can be summarized by the proper identification of 7 parameters (if neglecting outlet pressure drop). Based on these parameters and five independent inputs (the machine rotational speed, the fluid inlet and outlet pressures, the fluid supply enthalpy and the ambient temperature), the model computes the fluid outlet enthalpy, the shaft power and the fluid mass flow rate (as summarized in Table 1). It should be noted that sometimes the volume ratio is not known is therefore also becomes a calibration parameter. The parameters calibration can be performed using experimental measurements or manufacturer data, as well as simulation results from deterministic models. To this end, an optimization algorithm is used to calibrate the parameters $\boldsymbol{x}$ so as to minimize a global error residual $\boldsymbol{f}$ as given in Eq. (1). This equation is arbitrary (some weights are introduced for the three terms sometimes [11]).

$$\min_{\boldsymbol{x}} f = \sqrt{\sum_i \left(\left(\frac{\dot{m}_{meas,i}-\dot{m}_{pred,i}}{\dot{m}_{meas,i}}\right)^2 + \left(\frac{T_{meas,i}-T_{pred,i}}{\max(T_{meas})-\min(T_{meas})}\right)^2 + \left(\frac{\dot{W}_{sh,meas,i}-\dot{W}_{sh,pred,i}}{\dot{W}_{sh,meas,i}}\right)^2 \right)} \quad (1)$$

Table 1. Inputs, calibration parameters and outputs of the semi-empirical model

Inputs	Calibration parameters	Nomenclature	Outputs
Built-in volume ratio	Supply nozzle equivalent diameter	d_{su}	Shaft power [W]
Swept volume	Supply heat transfer coefficient	AU_{su}	Mass flow rate [kg/s]
Inlet temperature	Exhaust heat transfer coefficient	AU_{ex}	Outlet temperature [°C]
Inlet pressure	Ambient heat transfer coefficient	AU_{amb}	
Outlet pressure	Equivalent leakage area	A_{leak}	
Rotational speed	Proportional mechanical losses	C_{loss}	
Ambient temperature	Constant mechanical losses	α	
Clearance volume			

In practice, the reference database used for the parameters calibration (e.g. the measurements gathered on a test rig) does not necessarily cover the entire range of conditions onto which the model will be evaluated. For example, practical limitations of a test-rig may not allow to experimentally investigate the highest expander rotational speeds or the highest cycle pressure ratios. Therefore, the capability of the semi-empirical model to behave well in extrapolated conditions (i.e. in conditions out of its calibration domain) must be assessed to ensure reliable simulation predictions. This paper is dedicated to this topic and the next section describe a methodology to investigate the extrapolability of the expander semi-empirical model. The following analysis is performed in Matlab and the expander model can be downloaded in the open-access ORCmKit library [12].

2. Methodology to assess the model performance in extrapolation

Such a work has been done previously for compressors in 2015 [13] but the research is very limited for the case of expanders. In a previous paper, the authors investigated the extrapolation capability of various modelling approaches for the off-design simulation of ORC systems [14]. This analysis was performed for different system components, including a scroll expander and the semi-empirical model for volumetric machines investigated here. The extrapolability of the model was assessed by means of a cross-validation method in which the points used for the model evaluation (i.e. the test set) were defined *outside* of the training set (i.e. the reference points used for the model calibration). By means of a method extensively described in [14], the reference database was first plotted as a point cloud in function of the pressure ratio and the expander speed and then divided into two subgroups of equal size: an *internal* training dataset (used to calibrate the models) and an *external* testing dataset (used to cross-validate the models outside of the calibration domain). The results showed that the semi-empirical model is much more robust in extrapolation than polynomial regressions or constant-parameter models. The Mean Absolute Percent Error in extrapolation was equal to 5.52 for the expander power prediction and 1.6 for the mass flow rate (Fig. 2).

An issue with this approach is that it does not investigate the extrapolation conditions as generally met in practice. As presented here above, the method proposed in [14] uses as training set the points located in the “middle” of the database and assess the extrapolation performance of the model with the outermost points. In practice, however, a common problem with the experimental datasets is the absence of high rotational speeds and pressure ratios measurements while low values for these two parameters are easily obtainable. Therefore, in this paper, it is proposed to study the extrapolation performance of the expander semi-empirical model by using points with low pressure ratios and rotational speed as the training set and the rest of the reference database as test set.

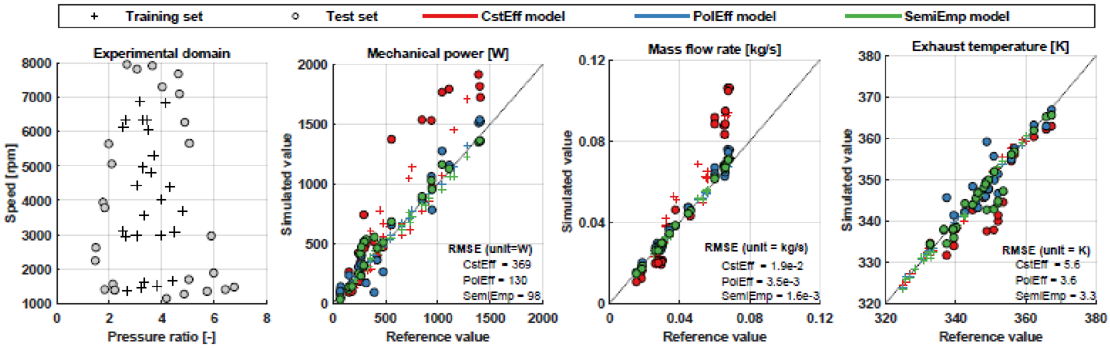

Fig. 2: Investigation of the extrapolation capability of various modelling approaches for the off-design simulation of ORC systems [13]. RMSe is the Root Mean Square Error.

To perform this work, an experimental database gathered on a 2kWe ORC system is used as case study (see [15] for further details on the test rig). The ORC unit includes a variable speed hermetic scroll expander and employs

R245fa as working fluid. The expander swept volume is 12.74 cm^3 and its volume ratio is 2.19. The range of operating conditions and the complete performance can be found in [16]. The methodology employed to characterize the extrapolation performance is as follows:

1. First, the experimental points in the database are sorted in function of their pressure ratio (resp. rotational speed).
2. Secondly, the selection of a training set is established with the points of the dataset are corresponding to a fraction of the pressure ratio (or rotational speed) range. It is accounted that the lowest pressure ratio (resp. rotational speed) corresponds to 0% and the highest to 100%. The training set is always composed of a minimum of 9 points to insure the acceptability of the calibration algorithm.
3. Then, the semi-empirical model is calibrated using points from the ***training set only*** (i.e. the points with a pressure ratio, or rotational speeds, lower than the specified threshold). The initial guess value for the parameters calibration is set equal to the optimal calibration with the full set of data.
4. Finally, the semi-empirical model is evaluated on the ***entire*** database and the Mean Average Error is computed for each of the three model outputs y_i (i.e. the mechanical power, the fluid mass flow rate and the exhaust temperature) with

$$MAE = \frac{\sum_{i=1}^{N} |\bar{y}_i - y_i|}{N} \tag{2}$$

where N is the total number of points, $\bar{y}_i$ is the reference output and y_i is the model output. The MAE is meaningful when we compare it to the actual value of the outputs. For this purpose, the mean value of the shaft power and the mass flow rate are 597 W and 0.042 kg/s respectively. The outlet temperature varies between 49°C and 95°C. The optimization algorithm used is the Patternsearch in Matlab. The comparison of different algorithm is out of the scope of this study.

3. Results

The methodology described in the previous section is first applied for 5 different calibration ranges (20%, 40%, 60%, 80% and 100%) in terms of pressure ratio. The evolution of the MAEs committed on the exhaust temperature, the shaft power and the mass flow rate predictions is depicted in Fig. 3. The analysis is performed using three different set of guess values for the parameters calibration (i.e. $x_{guess} = x_{opt}$, $x_{guess} = 300\%.x_{opt}$ and $x_{guess} = 600\%.x_{opt}$). From this graph, it can be seen that the mean average errors are very large only when the initial guesses are poorly chosen for the parameters calibration (i.e. $x_{guess} = 600\%.x_{opt}$) and when the calibration range covers solely over-expanded operating conditions (i.e. the maximum isentropic efficiency is not reached). Except for this particular situation, the extrapolation capability of the semi-empirical model appears to be very good and the MAEs are kept low even with narrow calibration ranges.

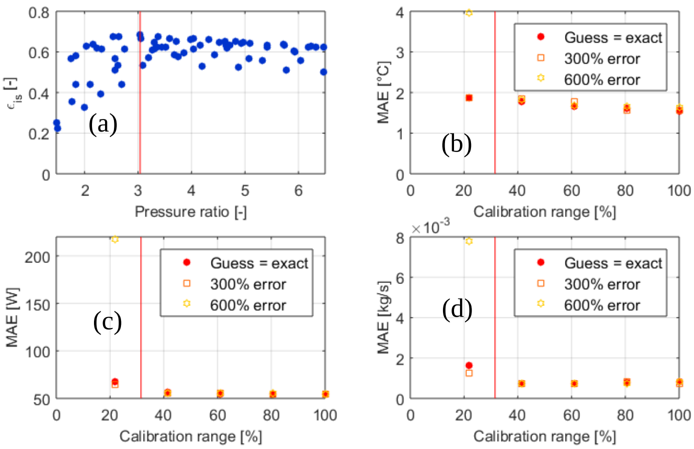

Fig. 3. Isentropic efficiency of the expander dataset as a function of the pressure ratio (a). Mean average error in extrapolation in function of the calibration range for the exhaust temperature (b), shaft power (a) and mass flow rate (d).

Figure 4 depicts the evolution of the calibrated parameters in function of the pressure ratio calibration range (in the case of well-posed guesses, i.e. $x_{guess} = x_{opt}$). These results correspond to the red points in Fig. 3. It can be seen that the parameters converge to stable values as the calibration range increases. The constant mechanical loss decreases while the proportional mechanical losses increase with a larger training set. Several local minima exists due to the large number of calibration parameters and sometimes, a combination of “wrong” parameters can lead to decent accuracy of the model outputs (there is not a global minimum for (1) but instead several local minima). In Fig. 4, it is shown that the MAEs are low (i.e. the model predicts well in extrapolation) even with 22% of the calibration range of pressure ratio. However, the parameters can have very different values from the optimal ones (100% range).

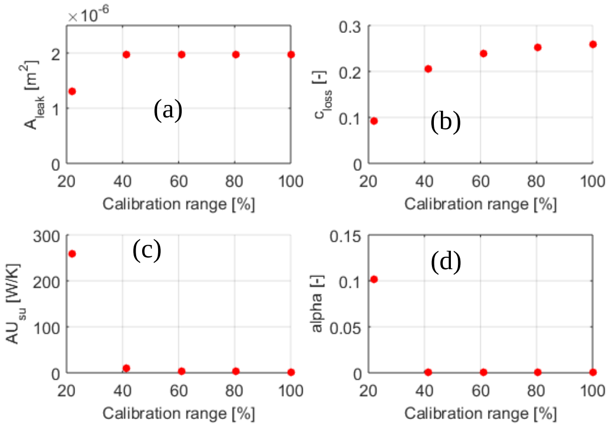

Fig. 4. Calibrated parameters with different calibration ranges. (a) Leakage area, (b) proportional mechanical losses, (c) supply heat transfer coefficient and (d) constant mechanical losses

The same analysis is then applied for 5 different rotational speed calibration ranges (20%, 40%, 60%, 80% and 100%). The evolution of the MAE evaluated on the three model outputs is shown in Fig. 5. Like before, the study is performed with three different guess values for performing the parameters calibration. The observations are similar for the rotational speed (Fig. 5) and for the pressure ratio (Fig. 3):): A too large error on the initial guess and a too small calibration range (<27%) leads to large MAE. But contrarily to the pressure ratio results, it appears that sometimes the MAE of a given output is smaller with a guess presenting a higher error. This is explained by the fact the only the sum of the square of the errors are minimized (1).

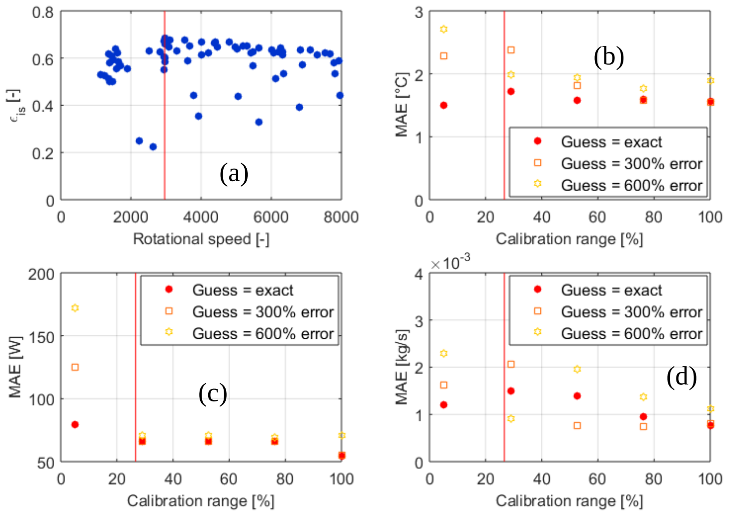

Figure 5: Isentropic efficiency of the expander dataset as a function of the rotational speed (a). Mean average error in extrapolation in function of the calibration range for the exhaust temperature (b), shaft power (a) and mass flow rate (d).

4. Discussion

Based on the results in section 3, it is possible to draw several guidelines to properly calibrate and use the semi-empirical model for volumetric expanders:

1. When calibrating the model with experimental measurements, it is recommended to experimentally explore the widest range of conditions to better assess the machine performance and to limit the extrapolation of the model in unseen conditions. At minimum, the training set should include over-expanded **and** under-expanded operating conditions so as to contain the machine maximum isentropic efficiency.
2. The selection of an accurate initial guess for the parameters calibration is mandatory if the training set misses points with high pressure ratios. If the training set includes points with both over-expanded and under-expander conditions, this constraint may be relaxed (i.e. a good estimate of the parameters values is not crucial).
3. Despite of the longer computational time, the parameters calibration should be performed with a derivative-free optimization algorithm in order to be less sensible to the parameters initial guesses and the presence of local minima in the residual function (1).

The best way to get reliable initial guesses for the parameters calibration is probably to perform a review of literature with experiments using the same technology of volumetric machine and fluid. However it is possible to approximate some parameters easily (neglecting supply and exhaust heat transfers, supply and exhaust pressure drops):

- The ambient heat transfer coefficient can be evaluated using an energy balance on the volumetric machine.
- The equivalent leakage area can be deduced from a flow conservation: the measured volumetric flow rate equals the leakage volumetric flow rate plus the theoretical volumetric flow of the machine.
- The mechanical loss coefficient(s) can be approximated assuming a given percentage of the isentropic power (e.g. 15%).

5. Conclusion

This paper proposes a preliminary study to assess the extrapolation capability and the limitations of a semi-empirical model for the simulation of volumetric expanders. The analysis is performed while using experimental data from a 2kWe scroll expander as case study. The extrapolation performance of the model is assessed through a cross-validation method. The results highlight the importance to have both under-expanded and over-expanded conditions in the training set to ensure a reliable calibration of the model. It is shown that by only using 41% of the maximum pressure ratio (resp. 27% of the maximum rotational speed), it is sufficient to get an accurate extrapolation (mean error lower than 5%). Ultimately, several guidelines are proposed to properly calibrate and employ this semi-empirical model.

A wide range of other cases should be tested following this methodology to generalize the results. The results could indeed be influenced by:

- The model itself: the semi-empirical model of an expander can presents various level of details. Some take into account (or not), an exhaust pressure drop, different laws of mechanical losses… and fifer in their modeling ([17,18])
- The considered volumetric machine: other power ranges, technologies, fluids and losses trends.
- The form of the objective function (1).

Those considerations should also be assessed in the case of semi empirical models of other components (exchanger, pump, compressor…). In a future work, the sensitivity of the model calibration to variations of the identified parameters in the same way as [18-20] should be done. Also, different approaches exist for this model

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