ZERO-DIMENSIONAL MODEL OF RECIPROCATING COMPRESSOR AND EXPANDER FOR A PHES SYSTEM

Wener N.*, Croza D., Favre F. and Curto-Risso P.L.
*Author for correspondence
Department of Applied Thermodynamics,
Universidad de la República - Faculty of Engineering,
Montevideo, 11300,
Uruguay,
E-mail: nwener@fing.edu.uy

ABSTRACT

One of the challenges of today is to achieve large amounts of electrical energy storage. This can be reached with the help of pumped heat energy storage (PHES) technology, where electricity is used to supply a heat pump system connected to two large thermal tanks. The system consists of four stages: compression, high temperature heat exchange (delivering in pump mode or absorbing in engine mode), expansion, and low temperature heat exchange (absorbing in pump mode or delivering in engine mode). From a technological point of view, the major issues to solve are the compressor and expander. Numerical simulations can be an important tool to quantify its theoretical potential. Numerous studies that simulate PHES systems use constant isentropic efficiencies to represent the compression and expansion stages. In this work a zero-dimensional model for a reciprocating compressor or expander is presented. Its objective is to represent the real behaviour of these stages and determine the main variables of the system. Therefore, a computer routine has been developed, which solves the system of differential energy equations and the mass balance as functions of the rotational speed. The model was validated using a domestic compressor and an industrial expander. To be able to reproduce the compressor case, a dynamic valve model that opens and closes according to the pressure of the system was implemented. In both cases a good agreement with experimental data from the literature was obtained.

With the present model, realistic values were obtained for the parameters that characterize the global irreversibility of the system, as well as their behaviour in relation to the crankshaft angle (or the elapsed time), an issue not usually well established in theoretical models. The dynamic model can be integrated in a PHES system simulation in order to represent its transient behaviour in a more realistic fashion.

INTRODUCTION

Nowadays, a large number of countries around the world make use of renewable energy, for example, from solar and wind sources. Due to the intrinsic variability of these phenomenon, energetic surpluses are expected and a flexible electric grid, capable of managing them, is necessary.

As previously mentioned, pumped heat energy storage (PHES) technology provides stability to the electrical system of a grid.

This work's main objective is to present a zero-dimensional model of a reciprocating machine, operating as a compressor or an expander, being capable of represent the real behaviour of them under non-standard operating conditions (characteristics of a PHES cycle) and to determine the main variables of its thermodynamic cycles.

In reference to the structure of the paper, a description of the analytical equations of a reciprocating machine model, including volume, mass, temperature and pressure, is first presented. Then the validation cases for both machines are described. Secondly, a methodology for calculating friction losses is proposed, in order to obtain the efficiency of the machines. Third, the results for the isentropic efficiency of the reciprocating machines are shown. Finally, a brief conclusion of the results is presented.

THERMODYNAMIC MODEL OF WORKING FLUID

A reciprocating machine, in its most simplified form, is a cylinder containing a piston (actuating as a variable wall) connected to a rod, which transmits force to the piston from the crankshaft (in the case of a compressor) or vice versa (in the case of an expansor). The following summarizes the model equations that describes the thermodynamic of the working fluid through these type of machine. [1]

The volume temporal derivative is presented below, obtained from geometric relationships between the piston linear position inside the cylinder and the angle of the crankshaft, φ:

$$\frac{dV}{dt} = \frac{V_0}{2}(r-1)\left(sen\varphi + \frac{sen\varphi cos\varphi}{\sqrt{\frac{1}{f^2} - sen^2\varphi}}\right)\omega \qquad (1)$$

where for simplification $f = a/l$ was defined as the geometric

NOMENCLATURE

φ	[rad]	Angle of the crankshaft
t	[s]	Time
V	[m^3]	Volume of the chamber occupied by the fluid
V_0	[m^3]	Minimum volume of the chamber
T	[K]	Gas temperature
p	[Pa]	Gas pressure
m	[kg]	Gas mass
r	[-]	Compression ratio
L	[m]	Stroke
a	[m]	Crankshaft radius
l	[m]	Length of the rod
f	[-]	Crankshaft radius and rod length ratio
γ	[-]	Gas adiabatic coefficient
C_p	[J/kg K]	Gas specific heat at constant pressure
C_v	[J/kg K]	Gas specific heat at constant volume
M	[-]	Mach number
v	[m/s]	Velocity of the gas through the nozzle
R	[J/kg K]	Ideal gas constant
A_T	[m^2]	Cross-sectional area
$\dot{m}$	[kg/s]	Actual mass flow through a nozzle
C_d	[-]	Choke coefficient through the nozzle
ρ	[kg/m^3]	Gas density
$\dot{W}$	[W]	Work performed by the system per unit of time
$\dot{Q}$	[W]	Heat flux between the cylinder body of the machine and the gas contained within
h	[J/kg]	Gas enthalpy
$\overline{P_p}$	[W]	Mean power for piston losses
μ_{oil}	[kg/m s]	Oil dynamic viscosity
A_c	[m^2]	Contact area between surfaces
$\bar{v}$	[m/s]	Root mean square velocity of the piston
H	[m]	Oil film thickness
$\overline{P_b}$	[W]	Mean dissipated power for bearing losses
D_c	[m]	Crankshaft diameter
ω	[rad/s]	Crankshaft angular speed
$\overline{P_f}$	[W]	Mean power loss due to friction
$\overline{P_i}$	[W]	Mean indicated power
$\overline{P_s}$	[W]	Isentropic power
$\overline{\dot{m}}$	[kg/s]	Mean weighted flow
$\overline{P_a}$	[W]	Mean actual power
$\eta_{is,e}$	[-]	Isentropic efficiency of an expander
$\eta_{is,c}$	[-]	Isentropic efficiency of a compressor

Special characters

x	[m]	Lift when obtained as a function of the angle of rotation
X	[-]	Relation between the angle of rotation and reference data taken from Ferrara *et al.* [6]

Subscripts

0	Initial condition
f	Final condition
dt	Total displaced
in	Intake
ex	Exhaust
j	Stagnation side
k	Side of the nozzle opposite to the stagnation point
min	Minimum
i	Discretization step i
$i+1$	Discretization step $i+1$
ss	Steady state
$2s$	State at the exhaust of a machine when an isentropic process is followed

relation between the crankshaft radius, a, and the length of the rod, l.

Applying mass balance to the cylinder, it is known that the temporal variation of the mass inside the chamber is determined by the intake and exhaust flows governed by the following equation:

$$\frac{dm}{dt} = \dot{m}_{in} + \dot{m}_{ex} \tag{2}$$

where $\dot{m}_{in}$ and $\dot{m}_{ex}$ are respectively the intake and exhaust flow, and m denotes the mass.

Therefore, it is necessary to study the intake and exhaust through the valves, which are dependent on the intake and exhaust pressures, as well as the fluid pressure inside the cylinder.

A nozzle flow model was assumed and the following definitions and hypothesis were used, in order to obtain both Eqs. (3) and (4) to represent the actual mass flow per unit of time through a nozzle when the Mach number is less than 1 and greater than or equal to 1, respectively:

- The heat per unit of mass transferred in the process can be neglected.
- The gas velocity at the intake is much lower than at the exhaust.
- The heat capacity of the fluid is considered as a constant value through the nozzle.
- p_j and T_j are the stagnation pressure and temperature respectively, while p_k and T_k are their counterparts on the other side of the nozzle.
- γ is the gas adiabatic coefficient, defined as $\gamma = C_p/C_v$.
- $M = v/\sqrt{\gamma RT}$ is the Mach number (denominator corresponds to the speed of sound and v is the velocity of the gas through the nozzle).
- The actual mass flow through a nozzle of cross-sectional area A_T is $\dot{m} = C_d \rho A_T M \sqrt{\gamma RT}$, according to [2], where C_d is the choke coefficient (which characterizes the passage through the nozzle) and ρ is the gas density.

For $M < 1$:

$$\dot{m} = C_d \frac{A_T p_j}{\sqrt{\gamma R T_j}} \gamma \left(\frac{p_k}{p_j}\right)^{\frac{1}{\gamma}} \left\{ \frac{2}{\gamma - 1} \left[1 - \left(\frac{p_k}{p_j}\right)^{\frac{\gamma-1}{\gamma}} \right] \right\}^{\frac{1}{2}} \tag{3}$$

For $M \geq 1$:

$$\dot{m} = C_d \frac{A_T p_j}{\sqrt{\gamma R T_j}} \gamma^{\frac{1}{2}} \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \tag{4}$$

The temperature temporal derivative was calculated applying the first law of thermodynamics to the control volume given by the working fluid contained in the cylinder. The following hypothesis and approximations were also used:

- The working fluid behaves as an ideal gas.
- The work per unit of time performed by the system was approximated by $\dot{W} = p\frac{dV}{dt}$.
- Single input (intake valve) and single output (exhaust valve).

$$\frac{dT}{dt} = \frac{1}{mC_p} \left[\dot{Q} + \dot{m}_{in} h_{in} + \dot{m}_{ex} h_{ex} - \frac{dm}{dt} h + \frac{dp}{dt} V \right] \tag{5}$$

In Eq. (5) T, m, h and p refers to the gas temperature, mass, enthalpy and pressure, respectively, and both h_{in} and h_{ex} refers to the intake and exhaust enthalpies. In addition, $\dot{Q}$ symbolizes the heat flux between the cylinder body of the machine and the gas contained within, and is calculated by means of the Adair's heat transfer correlation (described in [3]), developed for the study of reciprocating domestic compressors.

The pressure temporal derivative, dp/dt, is calculated using the ideal gas equation and the temperature time derivative shown in (5). The following expression was obtained:

$$\frac{dp}{dt} = \gamma p \left[\frac{1}{m} \frac{dm}{dt} + \frac{1}{mC_p T} \left(\dot{Q} + \dot{m}_{in} h_{in} + \dot{m}_{ex} h_{ex} - \frac{dm}{dt} h \right) - \frac{1}{V} \frac{dV}{dt} \right] \tag{6}$$

To resolve the dynamic operation of the alternative machine, a simulation routine was implemented using the C++ programming language and the equations previously presented. According to the last, a Runge–Kutta fourth-order iterative discretization method was used to obtain approximate solutions to Eqs.(2) and (5). [4]

Since the system is a cyclic process, it is easier to solve the differential equations using the angle as the independent variable, therefore the time derivatives previously shown were converted to angular derivatives using the chain rule.

Given an angular step i and the magnitudes m_i, T_i, p_i and V_i, it seems relevant to notice that the before mentioned discretization method was used only to obtain the gas' mass and temperature in the next step, $i+1$. Pressure in step $i+1$ is calculated by means of the ideal gas equation and the obtained m_{i+1} and T_{i+1}, as well as the volume V_{i+1}, which is calculated according to a geometrical relation (see [1]). The previous aims to mitigate the numerical error accumulated throughout the simulation.

Model validation for a compressor

The model of the reciprocating machine for the case of a compressor was validated using the example presented for Abidin *et al.* in [5]. In summary, this was based on the study of a domestic compressor model HTK55AA, using the refrigerant R-600a as the working fluid. Since this study considers the dynamics in the intake and exhaust valves, this phenomenon was additionally implemented for the validation of the model.

To simulate the dynamics of the valves, it is necessary to know the parameters that characterize their movement, that is: damping coefficient, spring stiffness, natural frequency of oscillation. In the reference case, this data is not provided, however, lift curves are presented as functions of the pressure difference, so it was decided to tune the model parameters by adjusting the lift curves obtained when comparing them against the reference. The latter is evidenced in Figure 1, where the comparison between the lift obtained and the reference case is shown.

Additionally, in the reference case, the modeling of the dynamics of auxiliary control volumes (such as mufflers on intake and discharge) was also included, since they affect the value of the compressor intake and exhaust pressures. To achieve results that fit the test conditions without needing to go into the modeling of these volumes, it was decided to obtain, from the reference data, the minimum value of pressure in the intake, and also impose a representative value of pressure in the discharge.

The input conditions (including those of the valves) and relevant output graphs are presented below, where the reference curves are attached where appropriate.

From the input parameters presented in table 1, Figure 2 stands out, which shows the comparison between the reference and what was obtained when using the model.

As can be notice, Figure 1 shows a well approximation of the dynamic behaviour of the valves, which is evidenced in Figure 2, where the pressure simulated shows a response almost identical of that of reference.

Table 1. Input parameters for compressor dynamic model validation.

Fluid	R-600a
Initial temperature and pressure	$T_0 = 63.6\ °C$, $p_0 = 62.60\ kPa$
Intake conditions	$T_{in} = 32\ °C$, $p_{in} = 59.16\ kPa$
Exhaust conditions	$T_{ex} = 116.85\ °C$, $p_{ex} = 620\ kPa$
Choke coefficients	$Cd_{ex} = Cd_{in} = 0.6$
Exhaust and intake valves diameter	$d_{ex} = d_{in} = 5.28 \times 10^{-3}\ m$
Angular velocity	$\omega = 308.92\ rad/s$
Piston diameter	$D = 21.1 \times 10^{-3}\ m$
Stroke length	$L = 15.4 \times 10^{-3}\ m$
Crankshaft length	$l = 33 \times 10^{-3}\ m$
Dead volume	$V_{min} = 85 \times 10^{-9}\ m^3$
Cylinder wall temperature	$T_{wall} = 82.8\ °C$
Coefficients of restitution	$e_{ex} = e_{in} = 0.4$
Exhaust valve parameters	damping $d = 0.5\ Ns/m$ spring stiffness $c_{ex} = 2000\ N/m$ natural frequency $f_{ex} = 8000\ Hz$
Intake valve parameters	damping $d = 0.005\ Ns/m$ spring stiffness $c_{in} = 600\ N/m$ natural frequency $f_{in} = 2300\ Hz$
Preload forces	$Fo_{ex} = Fo_{in} = 0.15\ N$

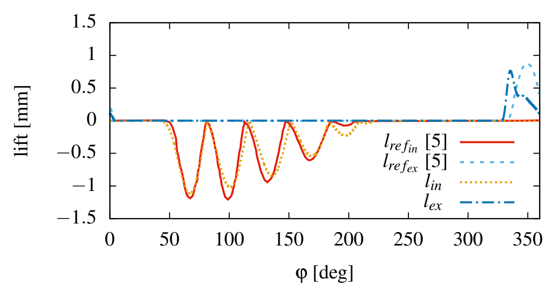

Figure 1. Comparison of lift obtained for intake and exhaust and the corresponding ones in reference [5].

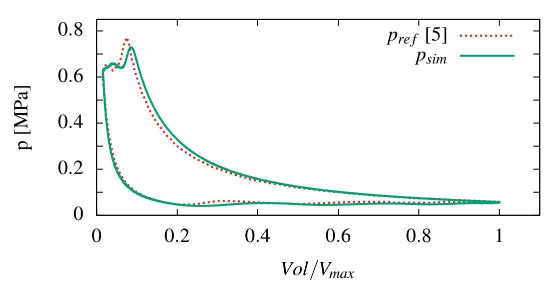

Figure 2. Indicated diagram comparison of the compressor.

Model validation for an expander

As for the compressor, the validation case for the expander model is presented. It should be noted that the models are practically identical (they start from the same equations), only changing the inputs (pressures and temperatures) and the opening and closing angles of the valves.

The reference case used was that of Ferrara *et al.*, presented in [6], which was based on the study of a reciprocating expander operating with steam.

In this case the operation of the valves follows the lift as a function of the angle of rotation. For the model, it was then decided to adjust it according to the lift curves provided in the reference case.

The following equations are used for the intake and exhaust lifts, respectively (obtained from the fit of the data provided in [6]):

$$x = \frac{4}{1000}\Big(1 - 0.3652X^{0.6319} - 1.084X^{1.277} + 0.4416X^{0.2854} - 0.0854X^{0.2843}\Big) \quad (7)$$

$$x = \frac{6}{1000}\Big(1 + 1.098X^{1.291} - 2.116X^{-1.471} - 0.09825X^{0.126} - 0.3161X^{2.558}\Big) \quad (8)$$

The input parameters to the program are presented in table 2 and the most pertinent output graph is presented below, in Figure 3, where the reference curve is attached.

Table 2. Input parameters for expander dynamic model validation.

Fluid	Water steam
Initial temperature and pressure	$T_0 = 90\ °C$, $p_0 = 100\ kPa$
Intake	$T_{in} = 160\ °C$, $p_{in} = 500\ kPa$
Exhaust	$T_{ex} = 86\ °C$, $p_{ex} = 60\ kPa$
Choke coefficients	$Cd_{ex} = Cd_{in} = 0.7$
Exhaust and intake valve diameter	$d_{ex} = d_{in} = 30 \times 10^{-3}\ m$
Angular velocity	$\omega = 240.86\ rad/s$
Stroke and piston size	$L = D = 72.6 \times 10^{-3}\ m$
Crankshaft length	$l = 134.4 \times 10^{-3}\ m$
Dead volume	$V_{min} = 15.8 \times 10^{-9}\ m^3$
Cylinder wall temperature	$T_{wall} = 100\ °C$
Max. intake and exhaust valves lift	$L_{in} = 4\ mm$, $L_{ex} = 6\ mm$

As can be seen in Figure 3, the results are well matched to those of the reference case, being both curves practically the same.

FRICTION LOSSES

A simple model is used to estimate friction losses that occur in the alternative machines (compressor and expander), as a function of geometric parameters of each machine, properties of

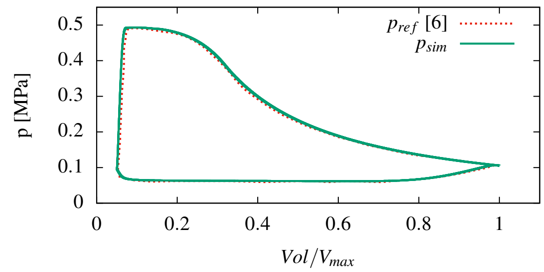

Figure 3. Indicated diagram comparison of the expander.

their lubricating oil and the rotational speed of the corresponding crankshaft.

The model takes only account for hydrodynamic friction, and considers two components of dissipated mechanical power: piston losses (including losses at the rings and the reminder of the piston walls) and bearing losses. These are the components that are taken into account in the consulted works, as the one of Lilie and Krueger in [7], or Dagilis and Vaitkus in [8]. It is assumed that contact between moving surfaces is through an oil coating with uniform thickness (eccentricity is not contemplated in neither of the movements). The lubricating oil is considered as a Newtonian fluid and the shear stress acting on the surfaces will be determined using the mean velocity gradient (relative velocity between the surfaces over oil film thickness) that occurs in each case.

For piston losses, under the mentioned hypotheses, the mean dissipated power is calculated according to Eq. (9):

$$\overline{P_p} = \frac{\mu_{oil} A_c}{H} \bar{v}^2 \quad (9)$$

Here, μ_{oil} stands for the oil dynamic viscosity, A_c for the contact area between the considered surfaces, $\bar{v}$ for the root mean square (RMS) velocity of the piston, which will be approximated by the mean piston velocity (twice the stroke over the time period that lasts one piston cycle), and H for the oil film thickness.

Eq. (9) applies to the piston rings (two rings are considered) and to the remainder of the piston wall.

For bearing losses, under the mentioned hypotheses, the mean dissipated power is calculated according to Petroff's law of friction, shown in tribology and/or lubrication textbooks, as [9]. This can be seen in Eq. (10):

$$\overline{P_b} = \frac{\mu_{oil} A_c \left(\frac{D_c}{2}\right)^2}{H} \omega^2 \quad (10)$$

Where D_c stands for the crankshaft diameter and ω for its angular speed.

Three bearings are taken into account for each cylinder.

Finally, from Eqs. (9) and (10), the mean power loss due to friction can be calculated by Eq. (11):

$$\overline{P_f} = \overline{P_p} + \overline{P_b} \quad (11)$$

CALCULATION OF ISENTROPIC EFFICIENCY

In this section, the calculation of the isentropic efficiency for a reciprocating compressor or an expander is presented.

Then, the variation of the isentropic efficiency of each machine with its angular velocity is shown in Figures 4 and 5, respectively for a compressor and an expander.

Additionally, the parametric variation of the efficiencies with the velocity ratio between the machines is presented in Figure 6.

The mean indicated power and the isentropic power are accordingly obtained from Eqs. (12) and (13), shown below.

$$\overline{P_i} = \frac{\omega}{2\pi}\int_{V(\varphi=0)}^{V(\varphi=2\pi)} p dV \tag{12}$$

$$\overline{P_s} = \overline{\dot{m}_{ss}}(h_{in} - h_{2s}) \tag{13}$$

with $\overline{\dot{m}_{ss}}$ being the mean flow in steady state, calculated as can be seen in (14), and h_{2s} being the enthalpy at the exhaust of the machine when an isentropic process is followed.

$$\overline{\dot{m}_{ss}} = \frac{|\ \overline{\dot{m}_{in}}\ | + |\ \overline{\dot{m}_{ex}}\ |}{2} \tag{14}$$

In the previous equation $\overline{\dot{m}_{in}}$ and $\overline{\dot{m}_{ex}}$ are the respective intake and exhaust mean weighted flows, obtained from the following equation:

$$\overline{\dot{m}} = \frac{\sum_{t_0}^{t_f} \dot{m}(t)}{N} \tag{15}$$

where N is the number of steps in a simulated cycle, and t_0 and t_f are the corresponding initial and final time. Conventionally, $t_0 = 0$ and $t_f = N\tau$, with τ being the temporal discretization step of each cycle.

The mean actual power of the machine can be obtained as follows in Eq. (16), resulting from the sum of the mean indicated power and the friction losses:

$$\overline{P_a} = \overline{P_i} + \overline{P_f} \tag{16}$$

Finally, the isentropic efficiency of a compressor or an expander can be calculated respectively as follows:

$$\eta_{is,c} = \frac{\overline{P_s}}{\overline{P_a}} \tag{17}$$

$$\eta_{is,e} = \frac{\overline{P_a}}{\overline{P_s}} \tag{18}$$

In the case of a compressor, both $\overline{P_i}$ and $\overline{P_s}$ take a negative value if calculated as previously presented. On the contrary, if the machine is an expander both take a positive value.

About $\overline{P_f}$, according to the previous analysis its value takes a negative sign, meaning that the actual power needed by the compressor is greater than the indicated power, or that the actual power given by the expander is less.

Using the previous equations, an asymptotic behaviour of the compressor efficiency for each velocity is observed, evidenced in Figure 4. For example, at 500 rpm the asympotote is barely greater than 90 %, and is reached at a pressure ratio of approximately 25.

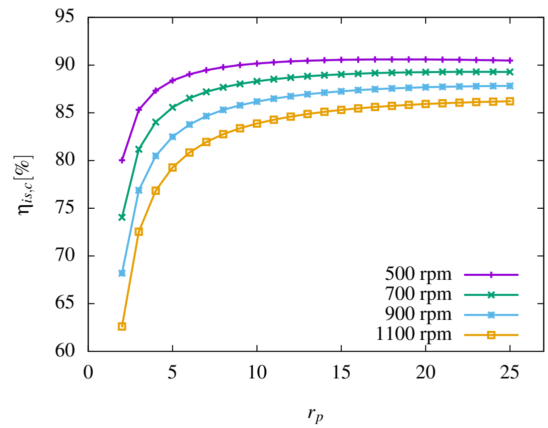

Figure 4. Compressor isentropic efficiency as a function of the pressure ratio. Parametric curves with the machine angular velocity are shown.

For the expander, a different behaviour can be noted, observed in Figure 5, where the curves present always a maximum of efficiency at a minor pressure ratio, which moves toward slightly greater ratios as the expander velocity increases.

Moreover, for both machines the isentropic efficiency drops as its velocity raises. This is evidenced in Figures 4 and 5.

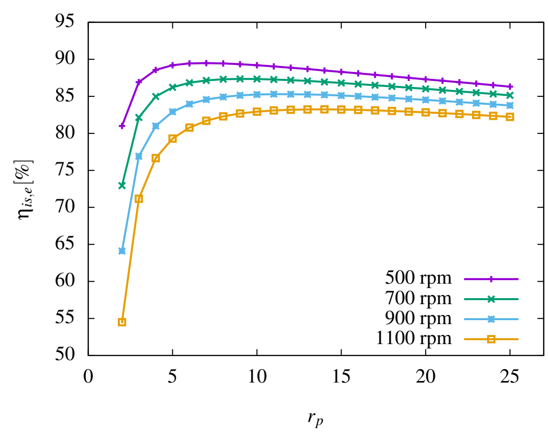

Figure 5. Expander isentropic efficiency as a function of the pressure ratio. Parametric curves with the machine angular velocity are shown.

Finally, the results shown in the previous figures are resumed in Figure 6, where the relation among the efficiencies of the machines is plotted as it varies with the pressure ratio, and also parametric with the velocity ratio between the machines, calculated as N_{comp}/N_{exp}. A velocity of 1000 rpm was used for the compressor, varying only the velocity of the expander to obtain the three velocity ratios plotted.

The net power consumed between the two machines, $P_n = P_c - P_e$, is added in certain points of each curve in Figure 6. P_c stands for the actual power consumed by the compressor and P_e for the actual power given by the expander, both considered positives in the previous calculation of P_n. It seems relevant to notice that the curves presented another tail at lower compressor efficiencies, but it was decided not to include it since given an expander efficiency, there were two possible points of the curve (corresponding to two different compressor efficiency, and therefore two different pressure ratios), and it is evident that it is preferable to work with the point of the highest compressor efficiency.

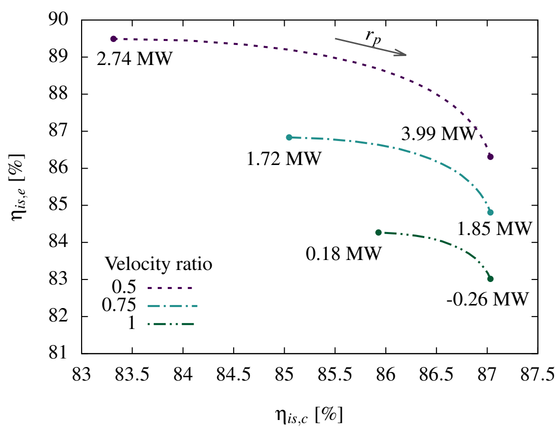

Figure 6. Efficiencies of the machines as functions of the pressure ratio and parametric with the velocity ratio. The net power corresponding to some points are also shown. Pressure ratio increases clockwise, with the final point of each curve at a ratio of 25.

From Figure 6 it can be noted that points with a higher pressure ratio present a better compressor efficiency, and also lead to a higher power consumption. In regard to the velocity ratio, it can be seen that the net power consumed by the system decreases when this ratio increases, even inverting the consume for certain pressure ratios when a relation of 1 is reached, being this type of working conditions evidently not suitable for a PHES system. Analogously to the asymptotic behaviour observed in Figure 4, the same response can be seen in Figure 6, evidenced by the vertical line followed by the points of the curves at a compressor efficiency of circa 87 %.

CONCLUSION

A thermodynamic model of the working fluid that circulates through a reciprocating machine has been implemented using a simulation routine in the programming language C++.

The implementation was validated using the reference cases of Abidin *et al.* [5] and Ferrara *et al.* [6], respectively for a compressor and an expander. The comparison between these references and the model simulation showed a well response for both machines, capturing the most relevant behaviours, evidenced in Figures 2 and 3.

To obtain the isentropic efficiency of each machine under different operating conditions (characterized by the pressure ratio and the angular velocity), a simple model to estimate the power loss due to friction was presented, based on the consulted works of Krueger and Dagilis and Vaitkus.

From the dynamic model and that of friction losses, the isentropic efficiencies of the machines were calculated. The obtained results were presented in Figures 4, 5 and 6, where it was shown the variation of each efficiency with both the angular velocity and the pressure ratio, and also the relation between both efficiencies when varying these two parameters.

In Figure 6 was also introduced the net power consumed between the machines, being possible to conclude that this power increases with the pressure ratio and decreases (even inverting its sign) with the velocity ratio.

Both in Figures 4 and 6 an asymptotic behaviour of the isentropic efficiency of the compressor was observed when the pressure ratio increases, this asymptote being decreasing with the angular velocity of the machine, and appearing at a pressure ratio close to 25.

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