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OPTIMAL HIGH PRESSURE CORRELATION FOR R744 DIRECT EXPANSION SOLAR ASSISTED HEAT PUMP FOR DOMESTIC HOT WATER

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Abstract. *Heat pumps can operate with a variety of refrigerant fluids. Among of them, the CO2 has excelled because of its favorable thermodynamics characteristics and zero net impact in climate change. The control of the gas cooler pressure is of utmost importance as it plays an important role in the system coefficient of performance (COP). In some research works it was proposed correlations to estimate the optimum high pressure, but none of them focusing solar assisted heat pumps. In this work it is presented a mathematical model of a Direct-Expansion Solar Assisted Heat Pump (DX-SAHP). This model was employed to investigate the influence of the high pressure on the system thermal performance. The results obtained from simulation were compared with the values estimated using correlations available in the literature. The mean difference of the optimum pressure found comparing both approaches was -25%. A new correlation was proposed in function of water flow rate and solar radiation rate. The mean difference of the optimum pressure obtained through simulations and by using the proposed correlation was 2.6%.*

Keywords: *R744, transcritical cycle, optimum high pressure, COP, solar assisted heat pump*

1. INTRODUCTION

In the past years, climate change have been one of a major worldwide concern. Many actions and efforts have been done to reduce greenhouse gas emissions. In this context, carbon dioxide (CO_2 or R744) as a refrigerant fluid become attractive to several researchers in the refrigeration area. Being a natural refrigerant, R744 has zero net impact in climate change. In addition, it is a not toxic, flammable or corrosive fluid, it is inexpensive and readily available fluid (Nekså, 2002).

However, one factor deserves attention when using CO_2 as a refrigerant fluid for heat pump systems. Due to its low value of critical temperature (31.1^{o}C) and its high pressure (73.7 Bar) to deliver heat at higher temperatures, the system has to operate in a transcritical cycle. Then, the control of the high pressure of a transcritical cycle becomes very important because this variable is directly related to the maximum coefficient of performance of the system.

Kauf (1999) proposed the first correlation to control the optimal high pressure as function of the refrigerant gas cooler outlet temperature. After that, many researchers investigated correlations for a single-stage R744 transcritical cycle as function of the refrigerant gas cooler outlet temperature or ambient temperature, such as Chen and Gu (2005) and Qi *et al.* (2013). Other authors as Yang *et al.* (2015) and Liao *et al.* (2000), proposed correlations for the optimal high pressure as a function of the refrigerant gas cooler outlet temperature and evaporation temperature. Wang *et al.* (2013) and Sarkar *et al.* (2006) also determined some correlations in terms of water temperature. Aprea and Maiorino (2009), besides the water temperature, included in their correlation parameters such as evaporation temperature, isentropic compressor efficiency and the gas cooler outlet temperature.

It can noticed that some properties are required to obtain the optimum high pressure correlation: as gas cooler outlet temperature, evaporation temperature, water inlet temperature, water outlet temperature and ambient temperature. Besides of that, the correlation can be modified with changes in the characteristic of the system components (Wang *et al.*, 2013). For a direct expansion solar assisted heat pump (DX-SAHP) the variation of solar radiation must be considered in the correlation model. The large energy input in the system promotes an increase in the evaporating temperature and the high pressure, resulting in a better coefficient of performance.

In the literature there a lack of works that investigated the high pressure correlation for a DX-SAHP, in that way, this paper presents a new correlation to calculate the optimal high pressure for these type of system. This correlation was developed using a mathematical model. In the end is presented a comparison between the proposed correlation with some existing others.

2. EXPERIMENTAL SETUP

The correlation is being developed to be employed in an existing DX-SAHP, that is installed at UFMG, Belo Horizonte (MG), Brazil. Figure 1 shows the main components at this DX-SAHP: two needle valve as an expansion device, an evaporator/collector, a reciprocating compressor, a liquid reservoir and a gas cooler. The refrigerant is carbon dioxide. This heat pump was developed to produce hot water for bath for a family of four people. The hot water is storage in a thermal energy storage with 200 Liters.

The CO_2 hermetic reciprocating compressor is manufacturer by Sanden and the model is SRcADB. The compressor has a swept volume of 1.75 cm^3/rev and it is driven by two 2 pole asynchronous electric motor (3500 rpm). The evaporator / collector and has a length of 1563.4$\pm$2.9 mm, width of 1000.4$\pm$3.3 mm the fin thickness are 0.55$\pm$0.02 mm. The evaporator tube has the length, the inner diameter and the outer diameter of respectively 16.3$\pm$0.13 m, 4.66$\pm$0.12 mm and 6.34$\pm$0.16 mm, and the distance between the tubes is 92.5$\pm$6.9 mm. The secondary fluid is air in the evaporator / collector. The length of the gas cooler CO_2 tube is 24.3 m. The counter flow gas cooler has the same diameters of the evaporator and the water tube has the inner diameter and outer diameter of respectively 10.52$\pm$0.15 mm and 12.5$\pm$3.3 mm. The material of the tubes in evaporator / collector and in the gas cooler are copper. The manual needle valve is manufacturer by Swagelok, model SS-31RS4 and has 1.6 mm of orifice diameter. The whole tube was insulated with 9 mm thick flexible insulation.

The operation range of the DX-SAHP are the ambient temperature is from 10 ^{o}C to 35^{o}C, and the water outlet temperature from 40 ^{o}C to 65 ^{o}C. The high pressure is from 71 bar to 90 bar.

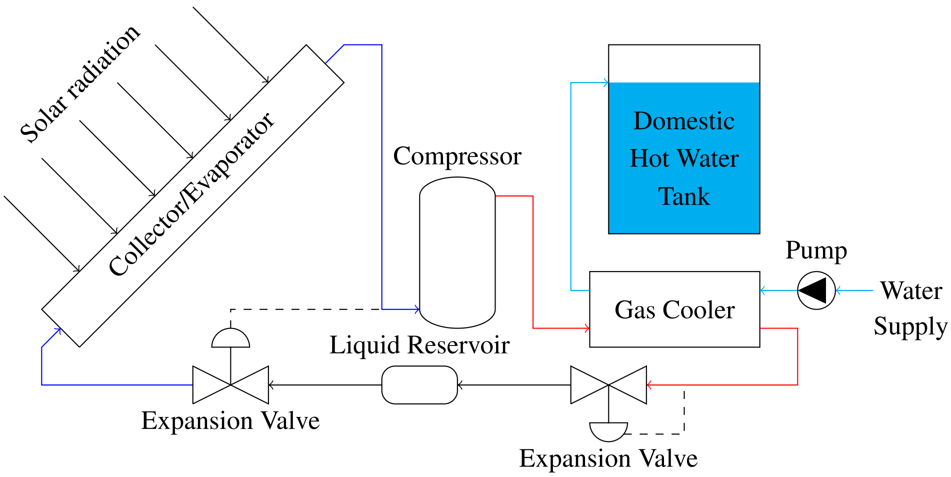

Figure 1. CO_2 DX-SAHP for heating water

3. MATHEMATICAL MODEL

In order to evaluate the performance of DX-SAHP for producing domestic hot water (DHW) a quasi-steady-state model was developed using the Equation Engineering Solver (EES). The losses in the tubes that connects the components was considered negligible. The evaporator/solar collector and gas cooler was assumed to be isobaric. A lumped model was used for the evaporator and a distributed model for the gas cooler. Following is described the mathematical model equations for each component.

3.1 Compressor model

The refrigerant mass flow rate ($\dot{m}_r$) for a constant rotation speed reciprocating compressor is given by:

$$\dot{m}_r = \rho_1 N V_s \eta_v \tag{1}$$

where ρ is the refrigerant density, N is the rotation speed, V_s is the compressor swept volume, η_v is the volumetric efficiency and the subscript 1 refers to compressor inlet or evaporator outlet. The compressor electric power consumption ($\dot{W}$), is evaluated as follow:

$$\dot{W} = \frac{\dot{m}_r(i_2 - i_1)}{\eta_g} \tag{2}$$

where η_g is the overall efficiency and i is the refrigerant specific enthalpy and the subscript 2 refers to compressor outlet or condenser inlet. The overall and volumetric efficiency was determined by fitting equations proposed by Minetto (2011) to the compressor performance map provided by the manufacture. The volumetric and overall efficiencies is given by:

$$\eta_v = -0.0922\left(\frac{P_2}{P_1}\right) + 0.9496 \tag{3}$$

$$\eta_g = -0.0069\left(\frac{P_2}{P_1}\right)^2 + 0.0234\left(\frac{P_2}{P_1}\right) + 0.4676 \tag{4}$$

where P is the refrigerant pressure.

3.2 Direct expansion solar evaporator model

The heat transfer rate received by the refrigerant in the evaporator ($\dot{Q}_{rev}$) is given by:

$$\dot{Q}_{rev} = \dot{m}_r(i_1 - i_4) \tag{5}$$

where the subscript 4 refers to thermostatic valve outlet or evaporator inlet. To evaluate the energy gain from air and solar radiation in a flat plate collector in steady-state condition, Kong *et al.* (2011) suggest the following equation:

$$\dot{Q}_{air} = A_e F'[aI - U_L(\overline{T}_r - T_a)] \tag{6}$$

where A_e is the area of solar evaporator, F' is the collector effectiveness factor, I is the solar radiation, a is the solar absorptivity, U_L is overall heat loss coefficient, $\overline{T}_r$ is the average temperature of the refrigerant fluid and T_a is the ambient air temperature.

The collector effectiveness factor proposed by Duffie and Beckman (2013), considering that the resistance to heat flow due the bond between the collector plate and tube can be neglected, is given by:

$$F' = \frac{1}{wU_{ev}}\left\{\frac{1}{U_L[D_o + F(w - D_o)]} + \frac{1}{\pi D_i h_i}\right\}^{-1} \tag{7}$$

where the distance between the tubes in the evaporator is w, the fin efficiency is F, the outer diameter is D_o, the inner diameter is D_i, the internal convective coefficient is h_i, that is calculated by the correlation proposed by Shah (2017) for two phase flow, and by the correlation proposed by Gnielinski (1976), for single phase flow. Shah (2017) presented a new correlation and compared the results with another seven correlations, using 4852 experimental data points from 81 sources and 30 different fluids including R744.

The fin efficiency can be evaluated by:

$$F = \frac{tanh\left[(w - D_o)/2\sqrt{U_L/(k\delta)}\right]}{(w - D_o)/2\sqrt{U_L/(k\delta)}} \tag{8}$$

where δ is the fin thickness and k is the thermal conductivity.

The overall heat loss coefficient proposed by Duffie and Beckman (2013) is determined by:

$$U_L = (h_{conv} + h_{cond} + h_{rad})_{bot} + (h_{conv} + h_{cond} + h_{rad})_{top} \tag{9}$$

where the subscripts bot and top represents the values at the bottom and top surface of the collector respectively. The convective coefficient (h_{conv}) is calculated by the correlation proposed by Kumar and Mullick (2010), the condensation convective coefficient (h_{cond}) from humid air is determined by the correlation proposed by Scarpa and Tagliafico (2016), the radiation heat transfer coefficient (h_{rad}) is given by:

$$h_{rad} = \varepsilon\sigma(\overline{T}_r + T_a)(\overline{T}_r^2 + T_a^2) \tag{10}$$

where the emissivity is ε, and the Stefan-Boltzmann constant is σ.

3.3 Gas cooler model

In the gas cooler model the following assumptions were made: (i) the thermal losses to environment and pressure drop are negligible; (ii) the properties of the walls, CO_2 and H_2O are equally distributed in the gas cooler section; (iii) thermal resistance of the wall tube due conduction is zero; and (iv) CO_2 and H_2O flow is one-dimensional. The energy balance for carbon dioxide, tube wall and water in any section of the gas cooler showed in Fig. 2, is given by:

$$\dot{m}_r \frac{\partial i_r}{\partial z} = h_r p_{ii}(T_s - T_r) \tag{11}$$

$$h_r p_{ii}(T_s - T_r) = h_w p_{oi}(T_w - T_s) \tag{12}$$

$$h_w p_{oi}(T_w - T_s) = -\dot{m}_w \frac{\partial i_w}{\partial z} \tag{13}$$

where p is the perimeter, z is the gas cooler position. Subscripts r, s and w refers to carbon dioxide, tube wall and water proprieties. Variables with subscripts ii, io and oi are geometrical parameter calculated with the diameters showed in Fig. 2. The convective coefficient h is calculated by the correlation proposed by Gnielinski (1976) for both, fluids and correct by Gosse (1981) factor for flow in annular region.

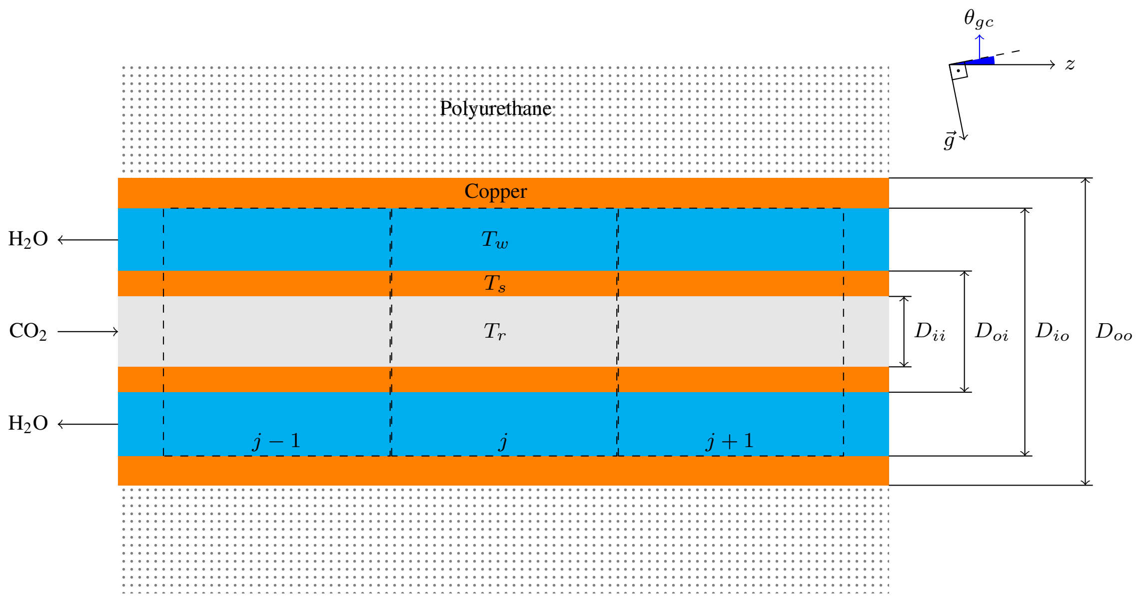

Figure 2. Gas cooler section geometry and control volume numbering

The boundary condition are the inlet temperature of water and refrigerant. To solve this system of differential equations, the finite volume technique and the central difference scheme descried by Versteeg and Malalasekera (2007) were used. This system of differential equations becomes the system of algebraic equations given by:

$$\dot{m}_r \frac{i_r(j) - i_r(j-1)}{\Delta z} = h_r p_{ii}[T_s(j) - T_r(j)] \tag{14}$$

$$T_r(j) = \frac{h_w p_{oi} T_w(j) + h_r p_{ii} T_r(j)}{h_w p_{oi} + h_r p_{ii}} \tag{15}$$

$$h_w p_{oi}[T_w(j) - T_s(j)] = -\dot{m}_w \frac{i_w(j) - i_w(j+1)}{\Delta z} \tag{16}$$

The enthalpy variables represent values at the outlet edge and the temperatures variable represent the values at the center of control volume. The simultaneous solution of the nonlinear system of equations would result in huge arrays with difficult convergence. An iterative solution is described by Machado (1996) that allow solve the equations for refrigerant and water separately. This iterative solutions is described in Fig. 3, where E_{tol} is a tolerance error, E_{Tr} is the refrigerant temperature convergence error and E_{Ts} is the wall temperature convergence error. This errors are given by:

$$E_{Tr} = \frac{T_r^p - T_r}{T_r} \cdot 100 \tag{17}$$

$$E_{Ts} = \frac{1}{n} \sum_{j=1}^{n} \frac{T_s^p(j) - T_s(j)}{T_s(j)} \cdot 100 \tag{18}$$

where the superscript p represents the value at previous iteration and n is the number of control volumes.

3.4 Heat pump model

The solution of the complete set of equations that constitute the mathematical model, considering a fixed water flow rate is also iterative and the flow chart used is showed in Fig. 4. The new values for evaporating temperature (T_4) is calculate by secant method described by Chapra and Canale (2008) in order to find the root of the error function. The errors introduced in Fig. 4 are given by:

$$E_{ev} = \frac{\dot{Q}_{rev} - \dot{Q}_{air}}{\dot{Q}_{air}} \cdot 100 \tag{19}$$

$$E_{T3} = \frac{T_3^p - T_3}{T_3} \cdot 100 \tag{20}$$

where the subscripts 3 represent the refrigerant properties at outlet of gas cooler. The superscript c and d represents the values calculated and desired, respectively.

The heat pump coefficient of performance (COP) is defined as follow:

$$COP = \frac{\dot{Q}_{gc}}{\dot{W}} \tag{21}$$

and the heat received by water at the gas cooler ($\dot{Q}_{gc}$) is given by:

$$\dot{Q}_{gc} = \dot{V}_w \rho_w (i_{wo} - i_{wi}) \tag{22}$$

where $\dot{V}_w$ is the volumetric water flow rate and the subscripts wi and wo represent water properties at the inlet and at the outlet of gas cooler.

4. OPTIMAL HIGH PRESSURE CORRELATIONS

Two existing correlations for the optimal high pressure will be used to produce comparative results with the new correlation for a CO_2 DX-SAHP. First, the correlation proposed by Liao *et al.* (2000) given by Eq. (23). The domain of this correlation is: (i) the refrigerant outlet gas cooler temperature (T_3) between 30^{o}C and 60^{o}C; (ii) the evaporation temperature (T_4) between -10^{o}C and 20^{o}C; (iii) the optimal high pressure between 71 bar and 120 bar. Second, the correlation proposed by Yang *et al.* (2015) given by Eq. (24). The domain of this correlation is: (i) the outlet gas cooler temperature between 30^{o}C and 60^{o}C; (ii) the evaporation temperature between -10^{o}C and 20^{o}C; (iii) the water outlet temperature between 55^{o}C and 80^{o}C.

$$P_{opt} = (2.788 - 0.0157T_4)T_3 + 0.381T_4 - 9.34 \tag{23}$$

$$P_{opt} = 2.918T_3 + 0.471T_4 - 0.018T_4T_3 - 13.955 \tag{24}$$

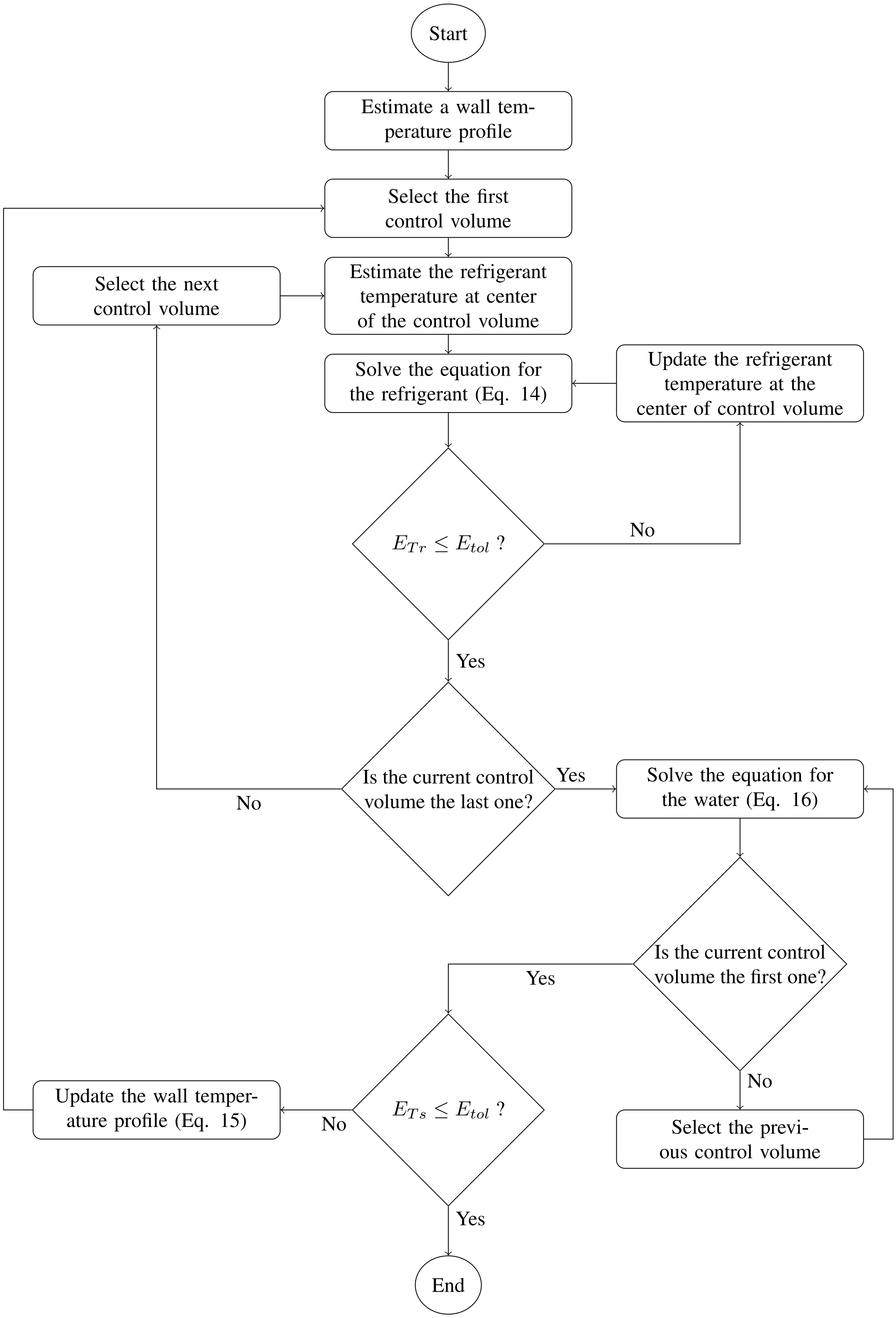

Figure 3. Flow chart for solving the gas cooler equations

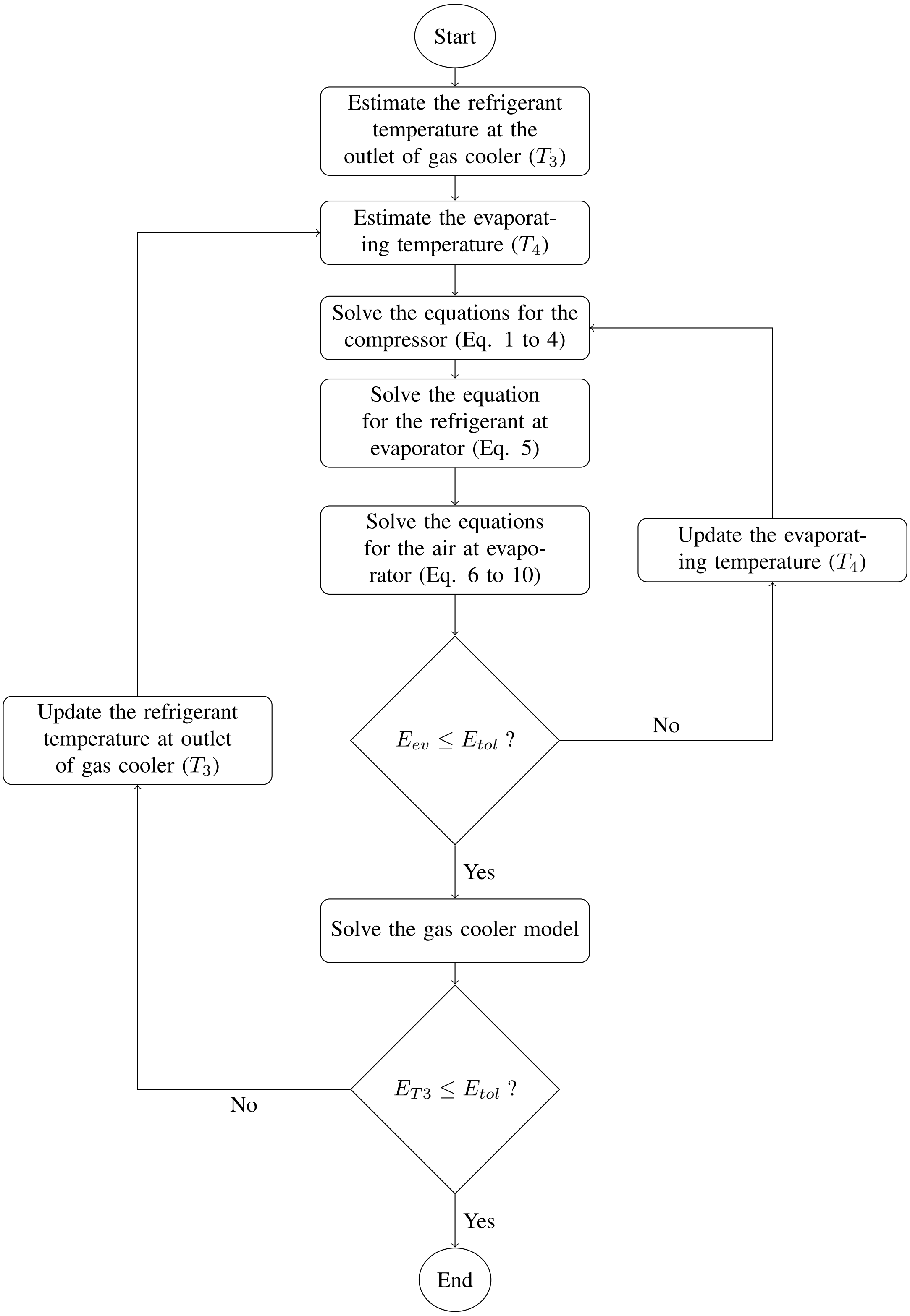

Figure 4. Flow chart for solving the equations of heat pump model

5. RESULTS AND DISCUSSION

5.1 Grid test

A spatial grid test was performed to determine the size of the control volumes in the gas cooler (Δz), following the directives described McHale and Friedman (2009). In this stage, two simulations was conducted: the first simulation was done considering the gas cooler pressure of 100 bar, ambient and inlet water temperature of 25^{o}C, no wind, a solar radiation of 500 W/m^2 and a water flow rate of 28.8 L/h. The second simulation was done considering the gas cooler pressure of 70 bar, ambient and inlet water temperature of 15^{o}C, wind speed of 2 m/s, a solar radiation of 800 W/m^2 and a water flow rate of 66 L/h. In both cases, for control volumes smaller than 110.5 mm, the changes in the values of COP and T_{wo} were smaller than the convergence tolerance error. Table 1 shows the results of the first simulation done in the grid test.

Table 1. Results of grid test for 100 bar, 25^{o}C, 0 m/s, 500 W/m^2 and 28.8 L/h

Δz (mm)	COP	ΔCOP (%)	T_{wo} (^{o}C)	ΔT_{wo} (%)
243	2.7072		75.292	
186.9	2.7376	-1.1	75.854	-0.7
143.8	2.7685	-1.1	76.428	-0.8
110.5	2.7958	-1.0	76.934	-0.7
85	2.8015	-0.2	77.040	-0.1
65.3	2.8122	-0.4	77.237	-0.3
50.2	2.8175	-0.2	77.335	-0.1

Then, after the spatial grid test, the following results were based in the list of parameters presented in Tab. 2 and the geometrical data listed in section 3. The carbon dioxide, water, air and copper properties were calculated using internal EES libraries.

Table 2. Simulations parameters list

Parameter	Value	Parameter	Value
Atmospheric Pressure	101.3 kPa	Relative humidity	70%
Emissivity	0.95	Solar absorptivity	0.95
Inlet water temperature	25 ^{o}C	Wind Speed	0 m/s
Ambient temperature	25 ^{o}C	Δz	110.5 mm
Superheat	10 ^{o}C	E_{tol}	$\pm$0.5 %

5.2 Influence of water flow rate in the COP

The COP, evaporating temperature, refrigerant and water outlet temperature are shown in Fig. 5 and 6 for different gas cooler pressure and water flow rate, for a solar radiation of 0 W/m^2. This solar radiation was chosen to check the accuracy of the correlation for optimum pressure available in the literature (Yang *et al.*, 2015; Liao *et al.*, 2000) since these correlations were developed considering an air source heat pump (ASHP). The maximum COP was reached at 90, 92, 94, and 98 bar for water flow rate of 25, 33.3, 28.6 and 40 L/h, respectively. The average difference between the optimum pressures found and calculated using the Liao *et al.* (2000) correlation is -22% and considering the correlation of Yang *et al.* (2015) the difference is -23%. Besides these large difference, these correlations are difficult to use in simulations since neither the evaporating temperature, nor the refrigerant outlet temperature remains constant if the pressure or mass flow rate changes. Therefore a specific correlation for a DX-SAHP should be developed.

The guideline of ASHRAE (2000) s a minimum temperature of 60^{o}C to minimize the risk of formation Legionellosis bacteria proliferation in the hot water storage, so an optimum mass flow rate to run the heat pump in ASHP mode is 33.3 L/h and the gas cooler pressure is 92 bar.

5.3 Influence of solar radiation in the COP

The COP, evaporating temperature, refrigerant and water outlet temperature are shown in Fig. 7 and 8, for different gas cooler pressures and solar radiations, considering a fixed water flow rate of 33.3 L/h. The maximum COP, for water outlet temperature higher than 60^{o}C, is reached at 92, 93, 98, 104, and 108 bar for solar radiation rate of 0, 200, 400, 600, and 800 W/m^2, respectively. The average difference between the optimum pressures found and calculated using the Liao *et al.* (2000) and Yang *et al.* (2015) correlations are -28%.

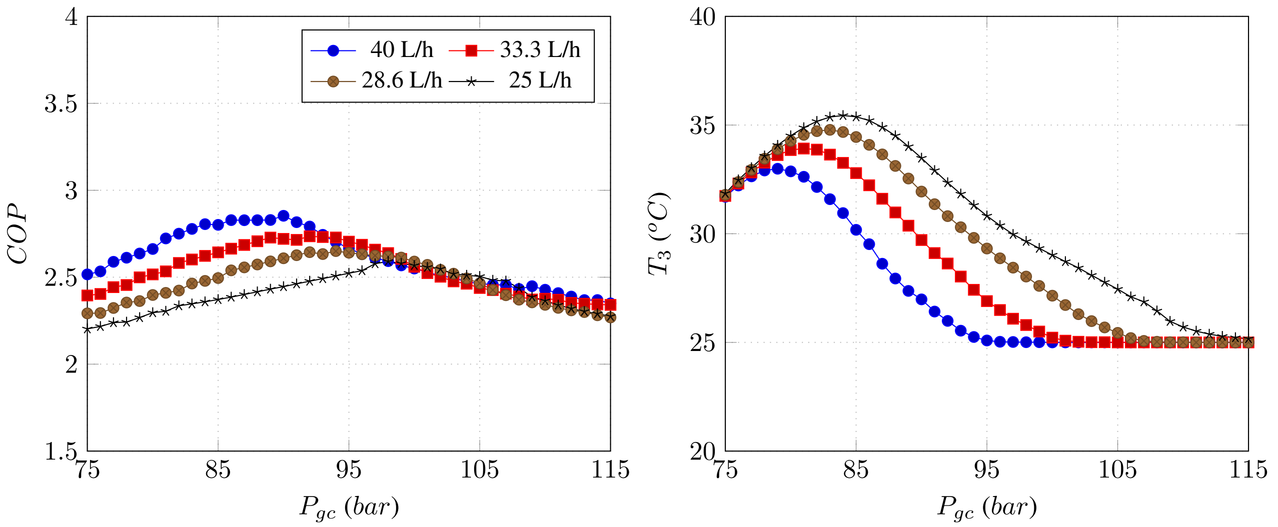

Figure 5. (a) COP regarding to gas cooler pressure and (b) refrigerant outlet temperature in the gas cooler (T_3) in function of gas cooler pressure for different water flow rate and a fixed solar radiation rate of 0 W/m^2.

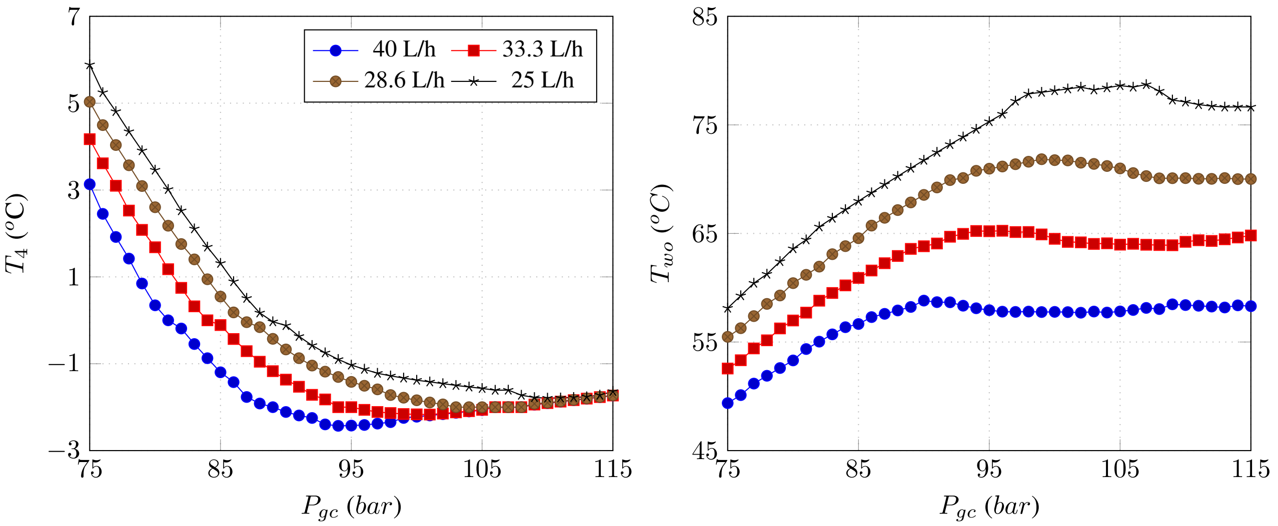

Figure 6. (a) Evaporating temperature (T_4) in function of gas cooler pressure and (b) water outlet temperature in the gas cooler (T_{wo}) in function of gas cooler pressure for different water flow rate and a fixed solar radiation rate of 0 W/m^2.

The discontinuity in the curves of 400 W/m^2 in the Fig. 7 and 8 for the pressure of 86 bar is due to the model converged for the pressure of 85 bar, with error of -0.48%, and for pressure of 86 bar with error of +0.47%, so this discontinuity can be eliminated running the model with smaller tolerance error. The same reason explain the discontinuity in the curves for solar radiation 400 W/m^2 and 92 bar. The causes of the discontinuities in the curves of 600 and 800 W/m^2 are due to the large variation of the thermal properties provide by EES close to the critical temperature (31°C).

5.4 Optimum pressure correlation

Twelve results of optimum COP, listed in Tab. 3, were divided in two data set. The first data set (DS1), tests 1 to 6, were used to fit the correlation and the second data set (DS2), tests 7 to 12, were used to check the accuracy of the correlation. The new correlation, based in the format of Eq. 25, was adjusted using the optimization Nelder-Mead Simplex method presented by Press *et al.* (1989) and the DIRECT method described by Gablonsky (2001), in order to minimize the Mean Absolute Difference (MAD) calculated by:

$$P_{otm} = C_0 + C_1 I + C_2 \dot{V}_w + C_3 \dot{V}_w I + C_4 I^2 + C_5 \dot{V}_w^2 + C_6 (\dot{V}_w I)^2 + C_7 I^3 + C_8 \dot{V}_w^3 + C_9 (\dot{V}_w I)^3 \tag{25}$$

$$MAD = \frac{1}{n} \sum_{n=1}^{6} \left| \frac{P_{sim} - P_{cor}}{P_{sim}} \right| \cdot 100 \tag{26}$$

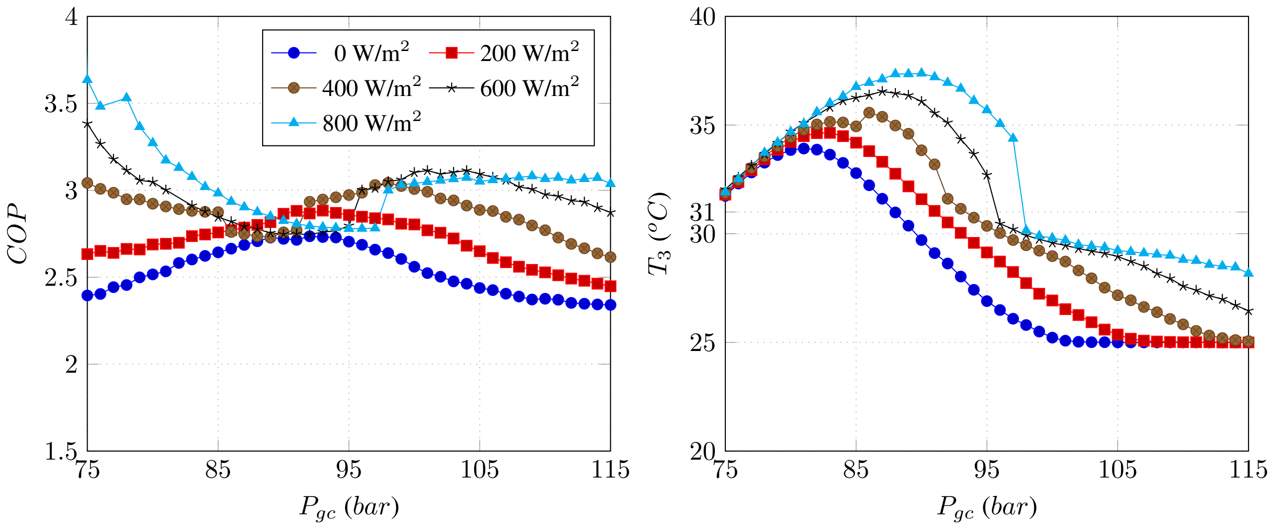

Figure 7. (a) COP regarding to the gas cooler pressure and (b) refrigerant outlet temperature in the gas cooler (T_3) in function of gas cooler pressure for different solar radiations and a fixed water flow rate of 33.3 L/h

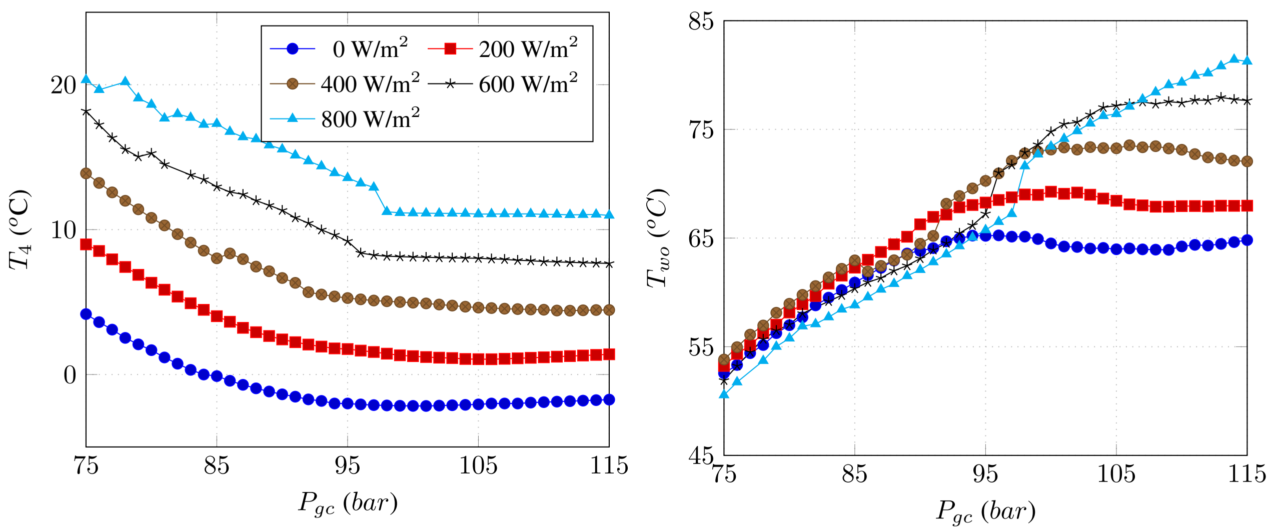

Figure 8. (a) Evaporating temperature (T_4) regarding to the of gas cooler pressure and (b) water outlet temperature in the gas cooler (T_{wo}) in function of gas cooler pressure for different solar radiations and a fixed water flow rate of 33.3 L/h

where the P_{sim} and P_{cor} represent the pressure found in the simulations and the pressure calculated by the proposed correlation, respectively. During the fitting process, only three constant from C_0 to C_9 were not null.

$$P_{otm} = 113.6 + 0.01957I - 0.5449\dot{V}_w \tag{27}$$

The best correlation found is describe in the Eq. 27. The MAD of the correlation considering the DS1 was 1.99%, considering the DS2 was 3.14%, and considering all results of Tab. 3, it was 2.57%. A graphical comparison between of the optimum pressure obtained from simulations and from correlation is presented in Fig. 9. This figure shows that the maximum difference between the optimum pressure calculated by the correlation and the value obtained from the simulation is 8%.

6. CONCLUSIONS

In this paper, an energetic analysis of a CO_2 DX-SAHP for producing domestic hot water was carried out using a mathematical model. The model was based in a heat pump equipped with a 1,6m^2 bare flat plate collector. The modeling was made using lumped model for the compressor, evaporator and expansion valve; and a finite volume model for the concentric counter flow gas cooler.

The results show that there is an optimum pressure for operating the R744 solar assisted heat pump in different solar radiation. Furthermore, the existing correlation was not good to predict the optimum pressure for a DX-SAHP and the

Table 3. Results of optimum COP

	Test	I (W/m^2)	$\dot{V}_w$ (L/h)	P_{gc} (bar)	COP	T_4 (°C)	T_3 (°C)	T_{wo} (°C)
DS1	1	0	25	90	2.85	-2.1	27.0	58.8
	2	0	33.3	92	2.74	-1.7	28.6	64.7
	3	0	28.6	94	2.65	-1.3	29.8	70.8
	4	0	40	98	2.59	-1.3	29.7	77.9
	5	200	33.3	93	2.88	1.9	30.0	67.8
	6	400	33.3	98	3.04	2.1	29.5	72.8
DS2	7	600	28.6	110	2.85	8.3	29.4	83.6
	8	800	33.3	109	2.59	11.1	29.0	79.1
	9	600	40	96	3.34	1.6	29.5	67.8
	10	600	33.3	104	3.11	1.5	29.1	77.0
	11	600	25	119	2.59	1.5	29.6	90.5
	12	400	28.6	106	2.85	5.1	29.0	81.2

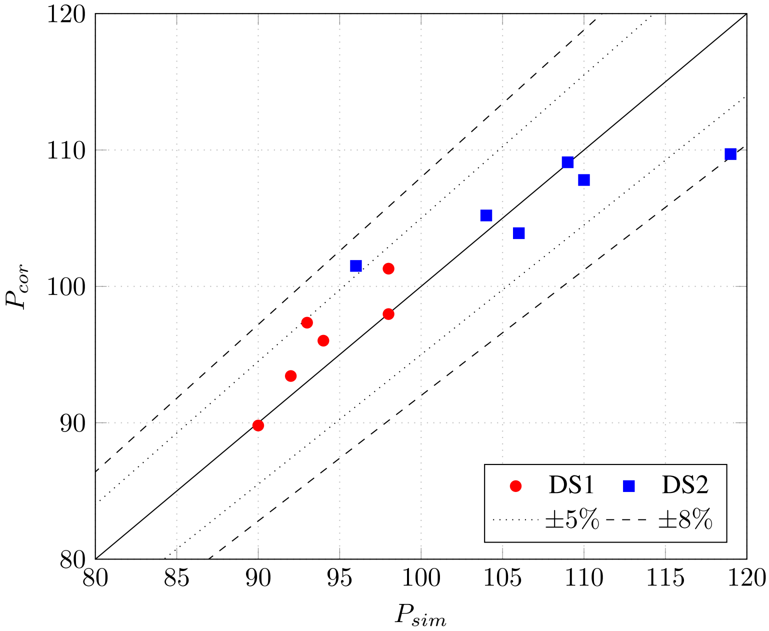

Figure 9. Comparison of Optimum pressure obtained from simulation and from new correlation

difference between the pressure calculated by the correlation extracted from the literature is about 22-28%.

A new correlation in function of solar radiation rate and water flow rate, was proposed. To fit and check the correlations 12 points of optimum COP were used. The mean difference and the maximum difference of the optimum pressure found in the simulations and provided by the new correlation is 2.57% and 7.8%, respectively.

7. ACKNOWLEDGEMENTS

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