

On-line LiBr+H₂O estimation for the performance of a water purification process integrated to an absorption heat transformer

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ABSTRACT

On-line LiBr+H₂O concentration is estimated and used to predict the coefficient of performance (COP) of a water purification process integrated to an absorption heat transformer (WP–AHT) applying a number of different algorithms developed in Matlab. The COP is a very important parameter for the performance of the WP–AHT. In this process the working fluid for the absorber and generator is LiBr+H₂O, whereas for the evaporator and condenser it is H₂O. The LiBr+H₂O is an important mixture to increase the energy in the absorber of the heat transformer. Two temperatures (absorber and generator) and two pressures (absorber and generator) are measured on-line to estimate the different concentrations of the absorber and the generator in steady-state on-line. An optimization method is taken to fit the unknown composition (X_{sol}) resulting from the equations. Through these on-line X_{sol} estimations, we can predict on-line COP values from a thermodynamic model. These results (X_{sol}) are satisfactory to estimate on-line the COP and to obtain the system operating conditions for each measured set of temperatures and pressures. Furthermore, with these algorithms that were developed, it is possible both to reduce costs of energy production and to allow a process control. Finally, the elapsed time to calculate the COP from this algorithm is 0.5 s, which is sufficient for the performance prediction of the system and it allows for automatic control.

Keywords: On-line LiBr+H₂O estimation; Water purification; Absorption heat transformer

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A B S T R A C T

On-line LiBr+H₂O concentration is estimated and used to predict the coefficient of performance (COP) of a water purification process integrated to an absorption heat transformer (WP–AHT) applying a number of different algorithms developed in Matlab. The COP is a very important parameter for the performance of the WP–AHT. In this process the working fluid for the absorber and generator is LiBr+H₂O, whereas for the evaporator and condenser it is H₂O. The LiBr+H₂O is an important mixture to increase the energy in the absorber of the heat transformer. Two temperatures (absorber and generator) and two pressures (absorber and generator) are measured on-line to estimate the different concentrations of the absorber and the generator in steady-state on-line. An optimization method is taken to fit the unknown composition (X_{sol}) resulting from the equations. Through these on-line X_{sol} estimations, we can predict on-line COP values from a thermodynamic model. These results (X_{sol}) are satisfactory to estimate on-line the COP and to obtain the system operating conditions for each measured set of temperatures and pressures. Furthermore, with these algorithms that were developed, it is possible both to reduce costs of energy production and to allow a process control. Finally, the elapsed time to calculate the COP from this algorithm is 0.5 s, which is sufficient for the performance prediction of the system and it allows for automatic control.

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1. Introduction

Absorption heat pumps are devices used for raising the temperature of low-grade heat to a more useful level using a smaller amount of relatively high-grade heat [1]. Applications range from residential to commercial and industrial needs; for example, in processes of heating, refrigeration, purification of effluents, etc. [2].

An absorption heat transformer is also known as a reversed absorption heat pump or temperature amplifier [1]. It delivers part of the heat input at a higher temperature and the rest at a lower temperature. Waste heat or solar thermal energy can be used as input heat for a single-stage heat transformer while the high-grade thermal energy delivered can be used as a heat source for water desalination. The absorption heat transformer is a system that consists of a thermodynamic device capable of producing useful heat at a thermal level superior to the

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one in the source [3]. In the energy cycle of an absorption heat transformer there are four main components: an absorber (AB), an evaporator (EV), a generator (or desorber) (GE), and a condenser (CO). The advantage of an absorption heat transformer is that it may be incorporated into any other process that requires a temperature greater than the one provided by the source.

In this context, several works report that it is possible to integrate the absorption heat transformer to a water purification process [2,4]. The integration of both processes makes it possible to increase the temperature of the impure water system, and thus it becomes useful for getting pure water and heat. An economizer is placed between the absorber and the generator to increase the efficiency of the cycle [5]. It differs from a conventional absorption heat pump in that the evaporator operates at a higher temperature than the condenser. It also employs two pumps instead of one [1]. The conventional heat transformer uses the LiBr+H₂O mixture, which is an ideal mixture for working pair [6]. The LiBr is the absorbent, whereas H₂O is the working fluid.

This research applies a configuration of an absorption heat transformer that increases COP by the incorporation of the waste-heat from the water purification condenser to both the absorption heat transformer evaporator and generator (see Fig. 1). This increase is obtained from the heat obtaining from the absorption heat transformer to be recycled, thus reaching a higher value of COP, while only the evaporator and generator temperatures are slightly increased [6, 7].

The value of the LiBr+H₂O composition is necessary to obtain the mass and energy balances to calculate the heat

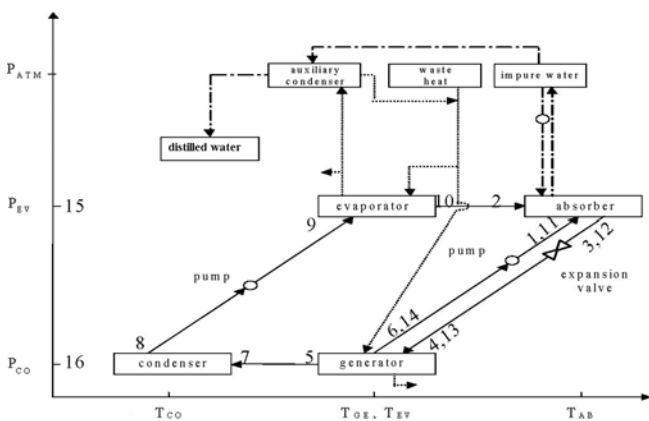


Fig. 1. Water purification process integrated to an absorption heat transformer with the incorporation of the waste heat from the auxiliary condenser to the evaporator and generator of the absorption heat transformer. Continuous line (—) represents the absorption heat transformer; interrupted line (---) represents the water purification process; dotted line (...) represents the recycled energy. Numbers that appear in some of the lines are the temperatures and pressures in the inlet and outlet of each component and which are measured.

flow rate of the generator and of the absorber in the internal primary circuit where the solution circulates. In addition, it is important to know the value of the concentration to avoid the proximity of crystallization of the solution under certain operations conditions; since this would involve severe damages in the components.

Consequently, the main goal of the present work is to on-line estimate the LiBr+H₂O concentration to predict the COP values based on the direct pressure and temperature measures in the integration of a water purification process to an absorption heat transformer with energy recycling. The thermodynamic model [6] is applied to predict the COP values within the internal circuit of the system. It is important to remark that in Escobar et al. [6], the pressures and concentrations were calculated from the literature because the pressures were not measured on-line.

2. Description absorption heat transformer integrated to a water purification process

Fig. 1 shows the diagram of the heat transformer waste energy recovery through the water purification process. The impure water tank takes heat from the absorber (Q_{AB}); this stream returns to the tank as a liquid-vapor mixture. The steam is sent to the auxiliary condenser where it is transformed to obtain distilled water. Then the resulting heat in the auxiliary condenser is recycled to the heat transformer.

2.1. On-line direct measures data acquisition

On-line direct measures, such as outlet temperatures of four components (AB, GE, CO and EV), as well as two pressures are carried out by robust sensors. A data acquisition system handles the signals. The on-line data acquisition system for the inlet and outlet temperature measurement of the fluids, and two pressures from absorber and generator in the absorption heat transformer integrated to the water purification process were applied. To get the data, we developed an algorithm in Matlab language and used the Agilent Virtual Instrument Software Architecture (VISA) which allows communication between computer and data acquisition equipment (Agilent 34970A), from the configuration of the port GPIB (General Purpose Interface Bus), and with the commands (fopen, fprintf, fscanf) of Matlab. GPIB is a digital communications bus specification whit parallel protocol to enable easier interconnection between data acquisition equipment and computer.

2.2. On-line LiBr+H₂O estimation considering the thermodynamic properties of the mixture

On-line LiBr+H₂O concentration is estimated by considering the correlation of the thermodynamic properties

of temperature, pressure and concentration of the LiBr+H₂O mixture, which is a function of the temperature (T) and of the pressure (P):

$$X_{\text{sol}} = f(T, P) \quad (1)$$

McNeely proposed an equation from the interrelation of these three properties [Eq. (1)] based on experimental information [3]. The author mentioned that the boiling temperature of the LiBr–H₂O solution (T_{sol}) is a function of the saturation temperature of the refrigerant fluid (T_{ref}) and of the mass composition X_{sol} of the LiBr–H₂O solution:

$$T_{\text{sol}} = T_{\text{ref}} \sum_{i=0}^3 A_i X_{\text{sol}}^i + \sum_{i=0}^3 B_i X_{\text{sol}}^i \quad (2)$$

where the saturation temperature of the refrigerant (T_{ref}) is a function of the saturation pressure (P_{sat}).

$$T_{\text{ref}} = T_{\text{ref}}(P_{\text{sat}}) \quad (3)$$

where A_i and B_i are constants of the McNeely equation. The domain of validity for the variables of Eq. (2) is the following: $-20^\circ\text{C} < T_{\text{ref}} < 110^\circ\text{C}$; $5^\circ\text{C} < T_{\text{sol}} < 180^\circ\text{C}$; and $45\% < X_{\text{sol}} < 70\%$ (% weight). The constants of the McNeely equation for the calculation of the boiling temperature of the the LiBr–H₂O solution, T_{sol} , appear in Table 1.

2.3. Thermodynamic model for COP prediction

The following assumptions have been made for the development of the thermodynamic model for an absorption heat transformer system (with reference to Fig. 1) [6]:

1. The entire system is in thermodynamic equilibrium.
2. The analysis is carried out under steady-state conditions.
3. A rectifier is not required since the absorbent does not evaporate under the operating temperature range of the system.
4. The solution that leaves the generator and the absorber is saturated; similarly, the working fluid leaving the condenser and the evaporator is also saturated.
5. Heat losses and pressure drops in the tubing and the components are considered negligible.

Table 1
Characteristic constant of the McNeely equation

i	A_i	B_i
0	-2.00755	1.24937E02
1	0.16976	-7.7165
2	-3.13336E-03	0.152286
3	1.97668E-05	-7.9509E-04

6. The flow through the valves is isenthalpic.

7. Outlet temperatures of the main components T5, T8, T10 and T3, and heat load in the evaporator Q_{EV} and generator Q_{GE} are known.

8. A heat supply is delivered by industrial waste heat.

From these assumptions it is possible to define the enthalpy-based coefficient of performance (COP) by the following equation [6]:

$$COP = \frac{Q_{\text{AB}}}{Q_{\text{GE}} + Q_{\text{EV}}} \quad (4)$$

where Q_{AB} , Q_{GE} and Q_{EV} are the heat flow rate (kW) for each one of the energy cycle components. These heats (Q s) are calculated from m , C_p , and ΔT for Q_{EV} and Q_{GE} and Eq. (8) for Q_{AB} .

2.4. Numerical solution

The estimation of the LiBr+H₂O concentration for the generator outlet was carried out from the thermodynamic properties of temperature and pressure. The pressure in the generator and the vapor temperature of the working fluid of the generator outlet represent the conditions of equilibrium of the LiBr+H₂O mixture.

$$X_6 = f(T_5, P_8) \quad (5)$$

The LiBr–H₂O composition in the generator inlet X_4 can be calculated by considering the optimization method (f_{zero} function of Matlab). Eq. (6) is solved in Matlab using a combination of bisection, secant and inverse quadratic interpolation methods to find the best values of X_4 , M_{GE} and M_{AB} that must satisfy mass and energy balance.

$$(M_{\text{WF}}H_5 + M_{\text{GE}}H_6 - M_{\text{AB}}H_4) - Q_{\text{GE}} = 0 \quad (6)$$

where

$$H_5 = f(T_5, P_5)$$

$$H_6 = f(T_6, X_6)$$

$$H_4 = f(T_4, X_4)$$

$$M_{\text{WF}} = \frac{Q_{\text{EV}}}{H_{10} - H_9}$$

where the mass flow rate value of the LiBr–H₂O solution in the generator inlet which comes from the absorber M_{AB} and the mass flow rate value in the generator outlet M_{GE} are obtained from the equations reported by Escobar [6]:

- Flow ratio:

$$FR = \frac{M_{AB}}{M_{WF}} = \frac{X_6}{X_6 - X_4} \quad (7)$$

where the mass flow rate of the working fluid flow is:

$$M_{WF} = \frac{Q_{AB}}{H_{10} - H_1 + FR(H_1 - H_3)} \quad (8)$$

and

$$M_{GE} = M_{AB} - M_{WF} \quad (9)$$

Q_{AB} is calculated based on M_{WF} [9].

3. Results and discussion

Fig. 2 shows the graphic interface of the direct measurement of temperature and pressure in the system. This figure presents the inlet and outlet temperatures of

every component of the water purification process integrated to an absorption heat transformer. These measured values are satisfactory since every component is working correctly, for example: the difference in the inlet and outlet temperature of the absorber is approximately 15°C. It is important to note that the pressures are only measurements in the generator and the absorber, and both the condenser and the evaporator pressures are considered similar to the ones from generator and absorber, respectively (see Fig. 2). An advantage of this graphic interface is that it can be manipulated in general form (for example, it is possible to stop the acquisition system to get changes in the measurements, it is possible to modified the graphic interface, it is possible to measure up to 66 variables, etc.). These values are applied in the thermodynamic model to calculate the COP. The outlet temperature of the auxiliary condenser (water purification process) is re-injected to the generator for energy recycling.

Fig. 3 shows a graphic interface of the measured values of temperatures and pressures, as well as the on-line estimation of the LiBr+H₂O concentration and of the COP values. Fig. 3 displays how the COP values are modified

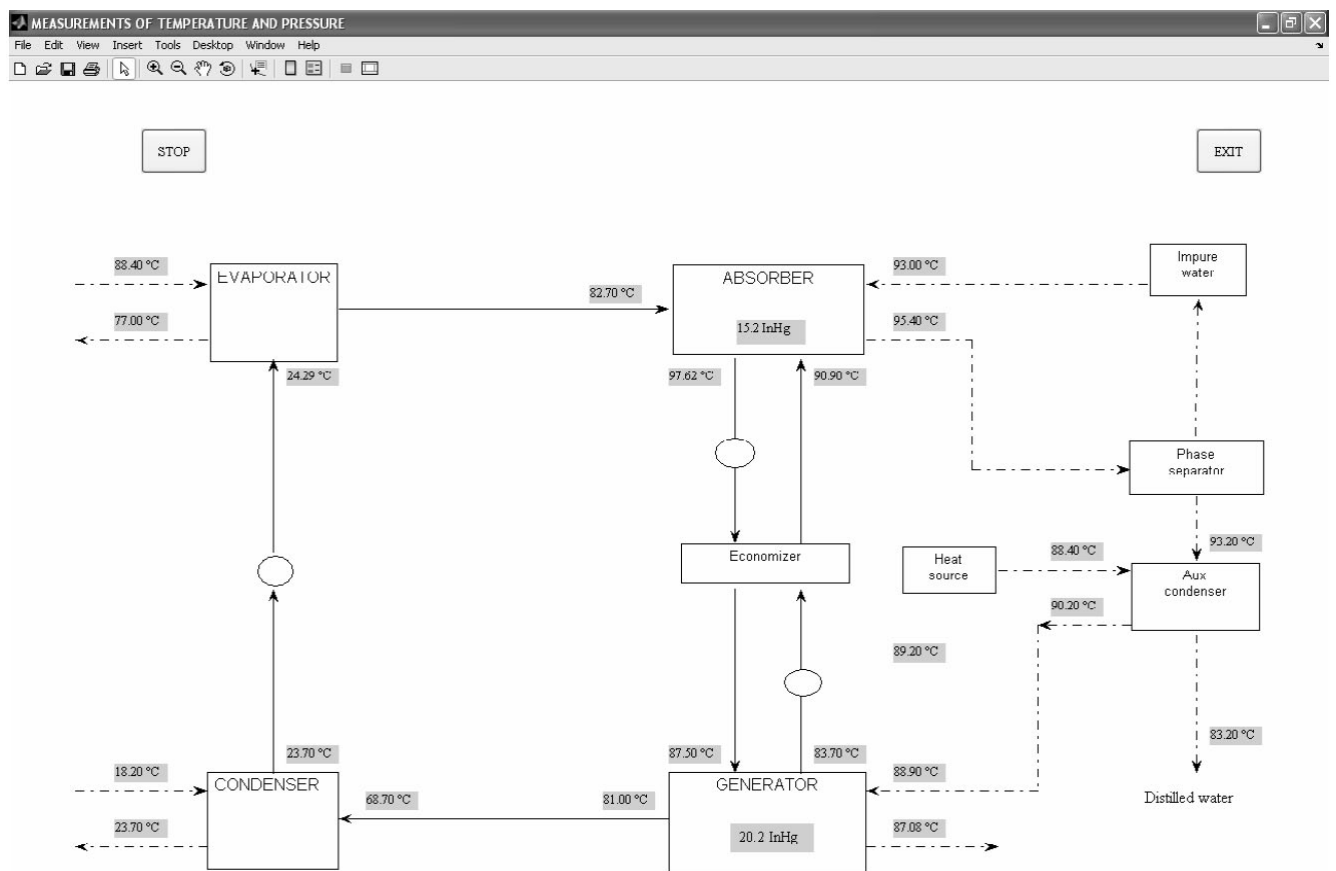


Fig. 2. Experimental data (temperatures and pressure) of the water purification process integrated to absorption heat transformer obtained from the data acquisition system.

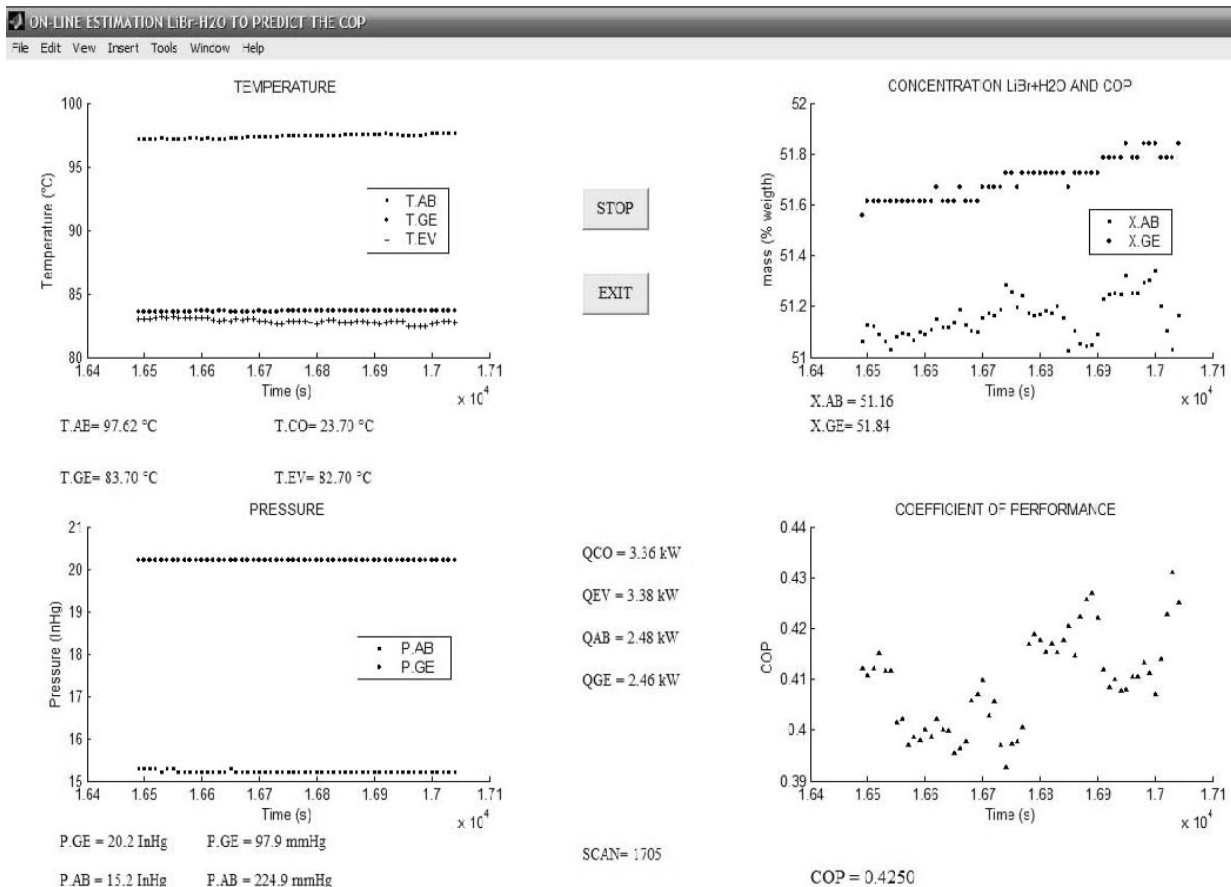


Fig. 3. Experimental data of temperature and pressure, as well as the on-line estimation of the LiBr+H₂O and of the COP values.

due to the changes of concentrations and pressures. Consequently, concentration and pressure are indeed key variables to calculate COP values. It is interesting to remark that similar results were reported in the literature considering the empirical model (neural network) [7,8]. Furthermore, we have to mention that Fig. 3 shows that the increase of the concentration in the generator also increases COP values. This is normal since the high concentration in the absorber inlet and the contact with the vapor result in a better absorption process. An additional advantage of this graphic interface remains in the fact that it can be manipulated in a general form (for example, it is possible to stop the acquisition system to get changes in the measurements, it is possible to modified the graphic interface, it is possible to measure up to 66 variables, etc.). And this advantage is very relevant when the inlet variables are modified during the process of simulation of the COP. This graphic interface allows us to observe the COP behavior for the system optimization.

3.1. Experimental data validation of the developed algorithms

The mathematical model and the developed algorithms for the LiBr-H₂O composition estimation and COP

values were validated through five tests carried out on the absorption heat transformer integrated to a water purification process reported by Bonilla-Peralta [10]. Table 2 shows that the values calculated for the LiBr-H₂O composition estimation for the generator outlet (X_{GE}) are similar to the experimental test. The values calculated for X_{GE} in the five tests presented an absolute maximum error of 1%. Table 3 shows that the LiBr-H₂O composition values calculated for the generator inlet which comes from the absorber (X_{AB}) are also similar to the experimental test. The studied values of X_{AB} for the five tests were obtained with an absolute maximum error of 1%.

Table 4 shows the difference between the experimental and simulated values of COP corresponding to the test. These differences can be due to energy loss that is not considered by the mathematical model [6] for the COP estimation. Nevertheless, real losses of heat exist in the absorption heat transformer. Moreover, the absorption process inside the absorber is another important factor to take into account, since the generated heat of the exothermic reaction, product of the absorption (water steam with the LiBr-H₂O solution) determines the useful heat flux of the absorber (heat retrieved and used for the process of water purification). The thermodynamic model

Table 2

Experimental and estimated values of X_{GE} for the different tests of validation of the model and the developed algorithms

Experiments	P_{GE} (mmHg)	T_{GE} (outlet condensator), °C	X_{GE} , experimental (% mass)	X_{GE} calculate (% mass)	Absolute error (%)
1	93.60	80.00	52.38	51.87	0.97
2	97.41	80.74	52.02	51.76	0.50
3	96.14	80.66	52.02	51.89	0.25
4	92.07	79.51	52.06	51.79	0.52
5	97.15	80.48	52.06	51.65	0.79

Table 3

Experimental and estimated values of X_{AB} for the different tests of validation of the model and the developed algorithms

Experiments	X_{AB} experimental (% mass)	X_{AB} calculate (% mass)	Absolute error (%)
1	51.56	51.19	0.72
2	51.39	51.23	0.31
3	51.39	51.18	0.41
4	50.89	51.32	0.84
5	50.89	51.12	0.45

Table 4

Experimental and simulated COP values for test validation of the model

Experiments	COP experimental	COP calculated	Absolute error (%)
1	0.2076	0.2679	29.05
2	0.2976	0.2352	20.95
3	0.2258	0.2453	8.65
4	0.3007	0.2497	16.95
5	0.2294	0.1863	18.74

that estimates the COP is only a theoretical approach from four real temperatures (AB, GE, EV, CO), two pressures (AB–EV and CO–GE) and two calculated concentrations (X_{AB} and X_{GE}). Furthermore, the thermodynamic model is obtained on base assumptions (heat losses and pressures drops in the tubing and into the components are considered negligible). Consequently, the difference between the experimental and simulated values demonstrates that it is necessary to work in the thermodynamic model so as to avoid to the assumptions (for example: to avoid heat losses in the system or to try to reduce pressure drops in the system and into the components to approach the thermodynamic model assumptions as close as possible).

4. Conclusions

The acquisition system developed for the direct measurement of temperature and pressure using the

MATLAB® software allows using the acquired information, for example, to the LiBr+H₂O concentrations estimate and COP values. This algorithm was developed with the Agilent BenchLink Data Logger software for the acquisition of information in the WP–AHT.

As for the mathematical model and the developed algorithms, it was possible to estimate the LiBr–H₂O composition and COP values because the time of calculation of the algorithm and the deployment of graphs on screen (0.53 s) are minor to the time of measurement of the variables (10 s). This on-line COP estimated can be used for the automation of the process. It was proved that it is feasible to obtain on-line the estimation for each time of measurement of temperature and pressure in steady state for the absorption heat transformer. The mathematical model appropriately represents the experimental information for the composition of the LiBr–H₂O solution during the operation of the absorption heat transformer in steady state. The model performs the estimation of the COP considering ideal conditions; therefore, values of major magnitude are obtained for the experimental values. In addition, the increase of the concentration in the generator also increases the COP values which is normal, since to major concentration in the inlet of the absorber and the contact with the vapor, the absorption is better carried out.

The system of information acquisition and the mathematical model present themselves as possible alternatives for the measurement of temperature and pressure during the operation of the absorption heat transformer and in the estimation of variables of interest that are not possible to measure in direct form.

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