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COEFFICIENT OF PERFORMANCE PREDICTION BY A POLYNOMIAL MODEL OF ABSORPTION HEAT TRANSFORMER

PREDICCIÓN DEL COEFICIENTE DE DESEMPEÑO POR UN MODELO POLINOMIAL PARA UN TRANSFORMADOR TÉRMICO

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Abstract

A polynomial model is developed to predict the coefficient of performance of a water purification process integrated to an absorption heat transformer. The range of the coefficient of performance operations was from 0.21 to 0.39. This model used: inlet temperature in the generator which comes from the absorber, outlet temperature in the absorber that comes from the generator, inlet temperature in the absorber that comes from the generator, water-lithium bromide solution inlet concentration in the generator that comes from the absorber and the pressure in the absorber and generator. A polynomial model is presented in order to obtain coefficient of performance prediction with a determination coefficient of 0.9919. Level surfaces of the coefficient of performance against the inlet variables for the polynomial model and residual analysis were presented with the aim of validating the model. This work has the purpose of providing faster and simpler solutions instead of the complex equations used for the analysis of the heat transformer in order to obtain accurate coefficient of performance prediction. The operation variable with the greater contribution of determination coefficient is presented.

Keywords: lithium bromide solution, residual analysis, Gaussian distribution, water purification.

Resumen

Un modelo polinomial es desarrollado para predecir el coeficiente de desempeño para un sistema de purificación de agua integrado a un transformador térmico. El rango de operación del coeficiente de desempeño fue desde 0.21 a 0.39. El modelo usa: temperatura de entrada en el generador el cual proviene del absorbedor, temperatura de salida en el absorbedor el cual proviene del generador, temperatura de entrada en el absorbedor el cual proviene del generador, concentración de entrada de la solución de bromuro de litio en el generador proveniente del absorbedor y la presión en el absorbedor y generador. Un modelo polinomial es presentado con el objetivo de predecir el coeficiente de desempeño con un coeficiente de determinación de 0.9919. Superficies de nivel del coeficiente de desempeño contra las variables de entrada del modelo polinomial y el análisis residual son presentados con el objetivo de validar el modelo. Este trabajo tiene el objetivo de proveer una solución rápida y simple en lugar de ecuaciones complejas usadas en el análisis del transformador térmico con el objetivo de obtener apropiadas predicciones del coeficiente de desempeño. La variable de operación con la mayor contribución en el coeficiente de determinación es presentada.

Palabras clave: solución de bromuro de litio, análisis residual, distribución Gaussiana, purificación de agua.

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1 Introduction

In linear multiple regression analysis, the goal is to predict, knowing the measurements collected from the data. In fact, the polynomial fitting is an attractive technique used for estimating the dependent variable in a system. The polynomial model has been used in several fields as: biomedical, environmental, socioeconomic studies Perez et al. (2009), composite dynamic envelopes thermal performance forecasting Lazaros et al. (2013) and electronic applications Hossain et al. (2011). Castilla et al. (2013) proposed the use of approximated models with the aim of reducing the computational cost required to compute the index, allowing its use in real-time control of systems and decreasing the size of the network sensor. The Authors compared an artificial neural network versus a polynomial model. Although, in general, the results obtained with the ANN model are better. The polynomial model can be derived in an easier way.

Absorption heat transformers which operate in a cycle opposite to that of absorption heat pumps can be used to reduce the CO_2 discharge and to reuse large amounts of industrial waste heat Horuz et al. (2009). Physical, theoretical and empirical models have been satisfactorily tested in order to model heat transformers and their components. Sencan et al. (2007) presented a comparison of different methods for modelling heat transformers powered by a solar pond. The coefficient of multiple determination R^2 value by: linear regression (0.26), pace regression (0.76), sequential minimal optimization (0.77), M5 model tree (0.52), M5' rules (0.51), decision table (0.25) and neural network methods (0.99), for the estimation of coefficient of performance. The comparison and methodology is based on experimental results by Rivera and Romero (1998). Siqueiros and Romero (2007) showed that proposed water purification coupled with a system absorption heat transformer is capable of increasing the original value of performance for more than 120% by recycling part of the energy from a water purification system by thermodynamic simulation. Hernández et al. (2008) and Hernández et al. (2009) developed a forecasting model for a water purification process integrated in an absorption heat transformer by direct and inverse artificial neural network with 16 variables in the inlet layer to obtain on-line prediction of coefficient of performance based on experimental results by Morales (2005). Sozen et al. (2007) analyzed the first and second laws of thermodynamics with the aim of evaluating an absorption heat transformer coupled to a solar pond operating with the aqua/ammonia, the maximum temperature of the useful heat produced was $\simeq 150\ ^oC$. Colorado et al. (2009) and (2011) described a physical-empirical model for a vertical helical evaporator and condenser under the heat transformer operation conditions. Juárez et al. (2009) presented a dynamic model to describe heat and mass transfer of a horizontal pipe absorber applied to a heat transformer used to purify water. Rivera et al. (2003) evaluated the theoretical integration between single and double stage absorption heat transformer with a distillation column of butane and pentane, the numerical results showed that it is possible to reduce the energy consumption in the re-boiler up to 43% by using a single stage heat transformer.

A heat transformer experimental rig has been studied by different authors. Rivera et al. (2011) applied the first and second law of thermodynamics to analyze the performance of an experimental heat transformer used for water purification. Results showed that decreasing the absorber temperature can lead to a better performance with low flow ratios and a greater amount of purified water. Sekar and Saravanan (2011) described an absorption heat transformer working with a water-lithium bromide solution coupled with a seawater distillation system. A maximum coefficient of performance of 0.38 and a maximum temperature lift of 20 ^oC have been reached under operation conditions, the quality of the water has been accepted as drinking water according to the Bureau of Indian Standard. Flores (2013) proposed a correlation for the heat transfer coefficient based on energy balance and Wilson plot method with experimental information of a double tube condenser under operation conditions of a heat transformer.

Actually, the integration of heat transformers with industry processes have demonstrated great interest. Moreover, engineers need more efficient tools to data processing and integration process assessment. As to the Author's knowledge, most of the theoretical inquiries regarding the absorption heat transformer modelling were carried out with complex empirical, semi empirical and thermodynamic assessment with satisfactory results. The aim of the present work discusses two main ideas; firstly, present a new methodology which provides faster and simpler solutions instead of the complex equations used for the analysis of the heat transformer in order to obtain accurate coefficient of performance prediction with a polynomial model and secondly, to determine the operation variable with the largest contribution to the determination coefficient of prediction. The polynomial model presented in this work was compared with an artificial neural network reported in the literature.

2 Experimental data

Figure 1 shows a schematic diagram of the absorption heat transformer integrated to a water purification process. The absorber gives us a useful heat quantity Q_{AB}, produced by the heat transformer from the evaporator, condenser and generator Siqueiros et al. (2007).

Experimental database provided by Morales et al. (2005) consists on different coefficient of performance values (COP), obtained from a portable water purification process coupled to an absorption heat transformer with energy recycling. An experimental data set was obtained at different initial concentrations of LiBr in LiBr + H_2O mixture, different temperatures in the absorber, the generator, the evaporator, and the condenser as well as different pressures in the absorber and the generator. Transitory and steady states were taken into account for each initial concentration of the mixture. After 2 hours from start-up, data was collected for 4 hours. Experiments were carried out at eight different initial conditions with at least two replicates. The arrangement was 8 + 2 with 4 hours of information acquisition. Thus, a database of 6786 samples was obtained. This data was sufficient for the polynomial model. A summary of the operating parameters is shown in Table 1.

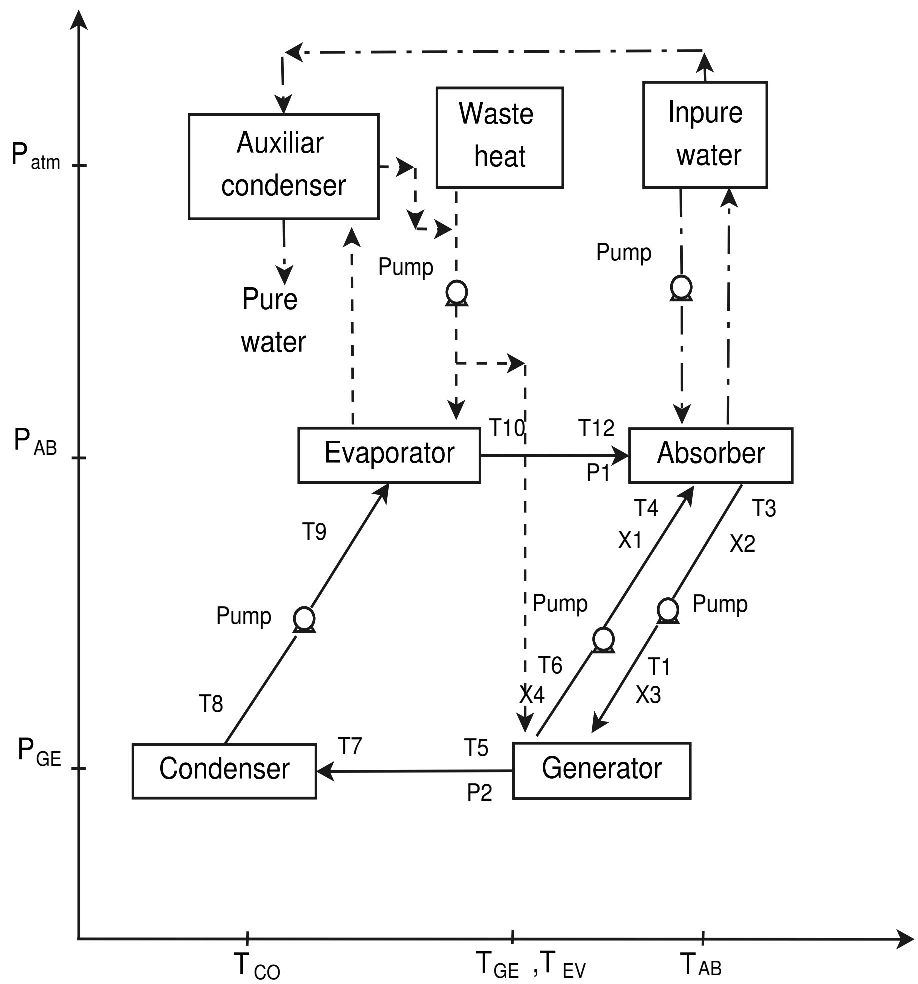

Fig. 1. Schematic diagram of absorption heat transformer integrated to water purification process with energy recycling.

Table 1. Range of experimental operating conditions used to obtain the coefficient of performance values

Temperatures (^oC)	Operation range	Instrumentation label (see Fig. 1)
$T_{in\ GE-AB}$	76.29-91.53	T1
$T_{in\ EV-AB}$	74.56-89.93	T2
$T_{out\ AB-GE}$	84.31-98.27	T3
$T_{in\ AB-GE}$	74.99-92.58	T4
$T_{out\ GE-CO}$	76.29-91.53	T5
$T_{out\ GE-AB}$	77.03-83.89	T6
$T_{in\ CO}$	40.37-65.03	T7
$T_{out\ CO}$	26.77-33.79	T8
$T_{in\ EV}$	28.52-85.33	T9
$T_{out\ EV-AB}$	74.56-89.93	T10
Concentrations (%)		
$X_{in\ AB}$	51.66-55.36	X1
$X_{out\ AB}$	50.75-54.36	X2
$X_{in\ GE}$	50.75-54.36	X3
$X_{out\ GE}$	53.16-56.07	X4
Pressure (*in Hg absolute*)		
P_{AB}	7.00-11.50	P1
P_{GE}	19.00-21.10	P2

Thermodynamic properties of the LiBr + H_2O mixture were estimated with Alefeld correlations cited by Torres-Merino (1997). The inlet and outlet-temperatures of each component (AB, GE, CO and EV) were obtained experimentally. At the same time, the pressure of two components (AB and GE) was registered with a temperature-pressure acquisition system (thermocouple conditioner and Agilent equipment with commercial software). Inlet and outlet-concentrations in the AB and GE were established by a refractometer (refraction index). In this process, LiBr + H_2O mixture was used as the working fluid in the absorber and generator, whereas only H_2O was used in the evaporator and condenser. A total of 16 variables (10 levels of temperature, 4 of concentration and 2 of pressure) were used and registered. Only the experimental database of an absorption heat transformer was used in this study.

2.1 *Experimental uncertainty analysis*

In the experimental rig, the quantities measured directly were: mass flow rate, pressure and bulk temperature. The rotameter, for the working fluid, had an accuracy of ±3% on the measurement. The manovacuometer uncertainty was estimated to be less than 0.5% of full scale, the scale of manovacuometer is from 0.033 bar to 2.07 bar. The measurements of thermocouples, T-type copper-constantan, had an accuracy of ±0.5 ^oC.

3 Methodology

In this section, the objective is to describe a methodology to build up a polynomial model that relates the coefficient of performance with the previous operation variables (see Table 1).

In general, relationship between the variables of interest, coefficient of performance and a number of associated (or inlet) variables $T1,\ldots,T10$, $X1,\ldots,X4$, $P1$ and $P2$ which are unknown but can be approximated by a polynomial model of the form:

$$\text{COP} = p(T1,\ldots,T10,X1,\ldots,X4,P1,P2)+\varepsilon, \quad (1)$$

where p is an unknown polynomial function and ε is the random error. It is assumed that ε is a random variable with Gaussian distribution.

To determine the polynomial model described in

Eq. (1), define the following predictor variable set:

$$A := \{Y_1, \ldots, Y_{16},\ Y_iY_j,\ Y_iY_jY_k,\ Y_iY_jY_kY_n,\ Y_iY_jY_k Y_nY_m | i = 1, \ldots, 16; j = i, \ldots, 16; k = j, \ldots, 16; n = k, \ldots, 16; m = n, \ldots, 16\}$$

where $Y_1 = T1, \ldots, Y_{10} = T10$, $Y_{11} = X1, \ldots, Y_{14} = X_4$, $Y_{15} = P1$ and $Y_{16} = P2$. As can be seen, it has to be checked with all combinations of variables up to polynomials of degree five, because polynomials with a degree greater than five only give a benefit of 0.0001 in the determination coefficient (R^2), a simple polynomial is required. The cardinality of set A equals to 51084,since that there are 16, 136, 2176, 9996 and 38760, terms of the form Y_i, Y_iY_j,$Y_iY_jY_k$, $Y_iY_jY_kY_n$, $Y_iY_jY_kY_nY_m$, respectively. Therefore, there are $2^{51084} - 1$ subsets of A without the empty set.

Linear multiple regression between A subsets and experimental coefficient of performance (COP) is used to find the simplest polynomial that fits the data. As you can notice, in the above paragraph, there are too many subsets of A, to discard some, the following criterion is used: if the coefficient of determination of Y_i and Y_i^n differed by less than 0.0001 then, Y_i^n is discarded ($n = 1, 2, \ldots, 5$). Under this criterion, it is easy to find the degrees of the monomials associated to the polynomial model in Eq. (1) (see Table 2.)

Table 2 shows that Y_{12} and Y_{13}, Y_1 and Y_5, Y_2 and Y_{10} have the same coefficient of determination, therefore, it can dispense with one of the two variables. Therefore the number of combinations that it needs to test is: $2^{13} - 1 = 8191$ (the products Y_iY_j,$Y_iY_jY_k$, $Y_iY_jY_kY_n$, $Y_iY_jY_kY_nY_m$ for $i \neq j \neq k \neq n \neq m$ were eliminated due to that provided few benefits to the coefficient of determination).

Then, the coefficient of determination is calculated (R^2) between each combination of variables and the coefficient of performance (COP) and the one with the highest R^2 coefficient is chosen.

4 Results

Remember that it seeks the simplest possible polynomial, therefore those with less variable polynomials are prefered. After trying many combinations:

$$\begin{aligned} COP \approx\ & 1.9123 \times 10^4 + 0.0247(T_{in\ GE-AB}) \\ & -0.0259(T_{out\ AB-GE}) + 0.0027(T_{in\ AB-GE}) \\ & -12.1769(X_{in\ GE}) + 0.1170(X_{in\ GE})^2 \\ & +1.0797 \times 10^3(P_{AB}) - 240.0364(P_{AB})^2 \\ & +26.4762(P_{AB})^3 - 1.4490(P_{AB})^4 \\ & +0.0315(P_{AB})^5 - 3.0444 \times 10^3(P_{GE}) \\ & +148.9803(P_{GE})^2 - 2.4298(P_{GE})^3. \end{aligned} \tag{2}$$

The fit of the polynomial model in Eq. (2) was expressed by the determination coefficient R^2 which was found to be 0.9919, indicating that 99.19% of the variability in the coefficient of performance could be explained by this polynomial model. Coefficient of performance can be seen as a linear combination of factors (see Table 3) plus an independent coefficient ($1.9223{\times}10^4$).

The polynomial (2) is not only the one with the highest determination coefficient, but also one of the shortest in terms of variables related.

Size of the confidence intervals (0.0004) (see Table 3) and coefficient of determination $R^2 = 0.9919$ shows that the monomials $T1, T3, T4, X3, X3^2, P1, P1^2, P1^3, P1^4, P1^5, P2, P2^2, P2^3$ have a linear relationship with the coefficient of performance (each treated as distinct and independent terms), to better appreciate this multivariable linearity see Figure 2. All the previously mentioned, supports the idea that the model is indeed valid.

Table 2. Monomials associated to our polynomial model.

	Variable	Degree	R^2
Y_1	$T1$	1	4.2078×10^{-6}
Y_2	$T2$	1	0.0934
Y_3	$T3$	1	0.0058
Y_4	$T4$	2	0.1977
Y_5	$T5$	1	4.2078×10^{-6}
Y_6	$T6$	2	0.1714
Y_7	$T7$	1	0.0550
Y_8	$T8$	1	0.0090
Y_9	$T9$	1	0.0096
Y_{10}	$T10$	1	0.0934
Y_{11}	$X1$	2	0.3121
Y_{12}	$X2$	2	0.3139
Y_{13}	$X3$	2	0.3139
Y_{14}	$X4$	2	0.1183
Y_{15}	$P1$	5	0.5488
Y_{16}	$P2$	3	0.1238

Table 3. Each coefficient are shown with their corresponding confidence interval with a confidence level of 99%.

Factor	Coefficient	Confidence Interval
$T1$	0.0247	[0.0245, 0.0249]
$T3$	-0.0259	[-0.0261, -0.0257]
$T4$	0.0027	[0.0025, 0.0029]
$X3$	-12.1769	[-12.2857, -12.0680]
$X3^2$	0.1170	[0.1159, 0.1180]
$P1$	1.0797×10^3	[1.0659×10^3, 1.0936×10^3]
$P1^2$	-240.0364	[-243.1142, -236.9585]
$P1^3$	26.4762	[26.1369, 26.8155]
$P1^4$	-1.4490	[-1.4676, -1.4304]
$P1^5$	0.0315	[0.0311, 0.0319]
$P2$	-3.0444×10^3	[-3.1268×10^3, -2.9620×10^3]
$P2^2$	148.9803	[144.9588, 153.0017]
$P2^3$	-2.4298	[-2.4952, -2.3644]

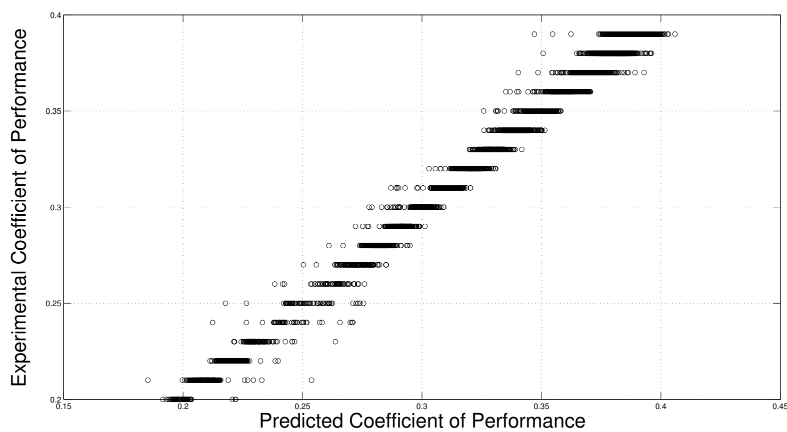

Fig. 2. Experimental versus predicted coefficient of performance for database.

On the other hand, remember that the variables involved in the polynomial (see Eq. (2)) are: $Y_1 = T1, Y_3 = T3, Y_4 = T4, Y_{13} = X_3, Y_{15} = P1$ and $Y_{16} = P2$, then to give a geometric idea of the behaviour of the polynomial predictor p, experimental and predicted coefficients of performance are plotted, however it is noteworthy that the polynomial has six different variables therefore, level surfaces are plotted for each variable, the two-dimensionals and three-dimensionals are later shown in Figures 3, 4 and 5. As can be seen, there is good agreement between predicted values and experimental data points.

4.1 Residual analysis

In this subsection, a residual analysis to verify the goodness of the polynomial fit in Eq. (2) is presented by Montgomery (2001) and (2010) and by Devore (2004).

In section 4, it is supposed that in Eq.(1), ε had a Gaussian distribution. Under assumption that ε has a zero mean, the expected value (E) can be taken on both sides of the equation (1) as follows:

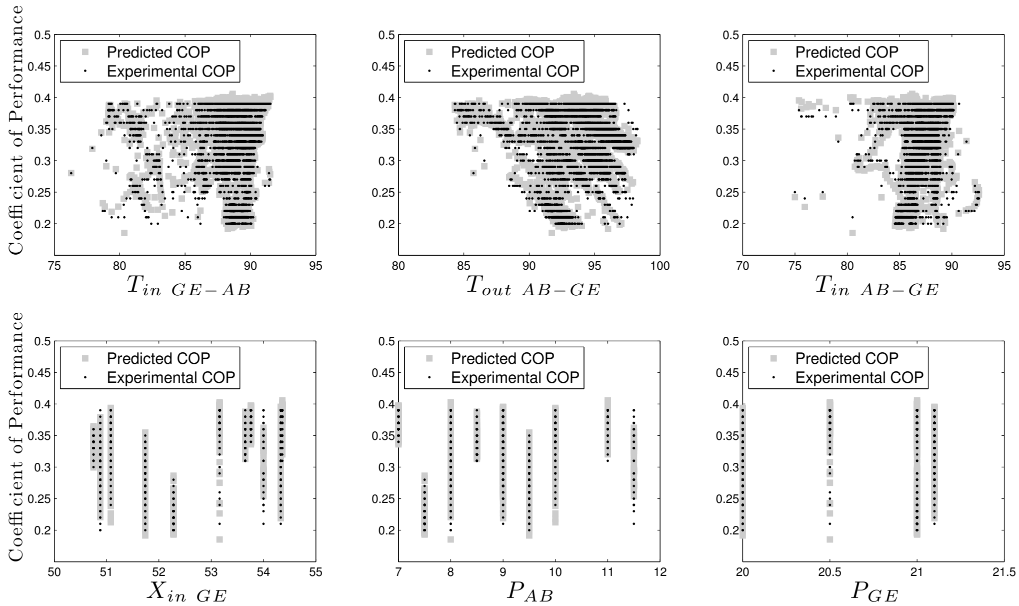

Fig. 3. Level surfaces. Comparison of experimental and predicted coefficient of performance for each variable significant in the polynomial model.

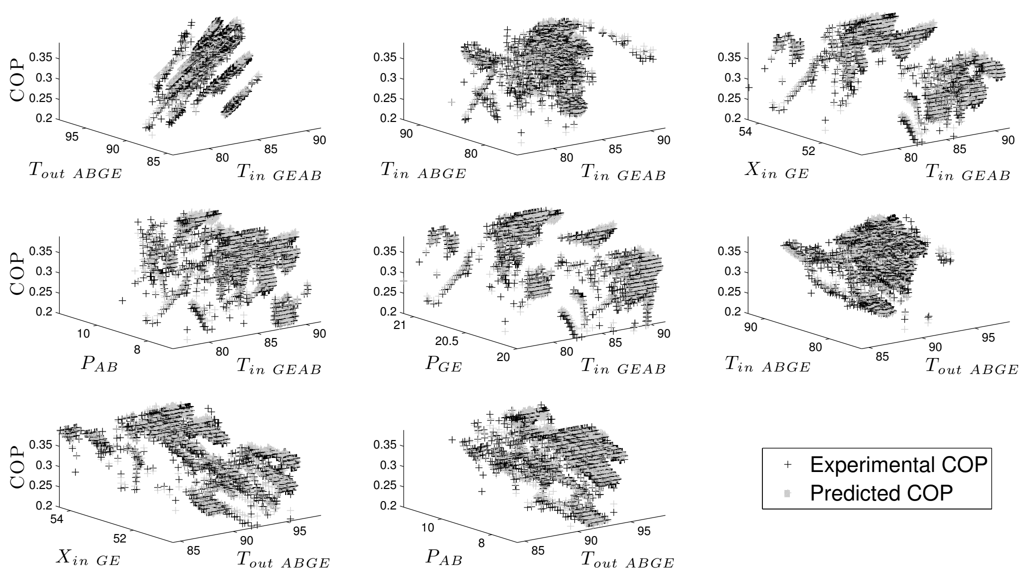

Fig. 4. Level surfaces. Comparison of experimental and predicted coefficient of performance for each two variables significants in the polynomial model.

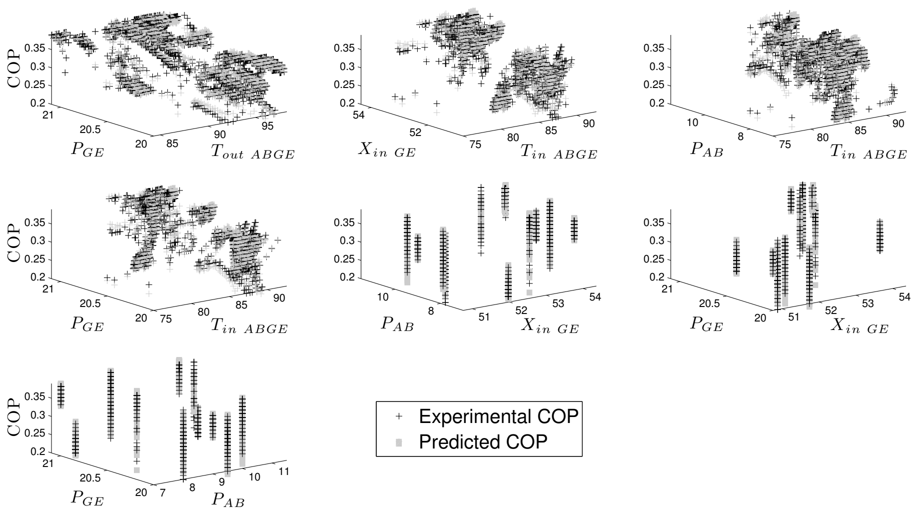

Fig. 5. Level surfaces. Comparison of experimental and predicted coefficient of performance for each two variables significants in the polynomial model.

$$
\begin{aligned}
E(COP) =& E(p(T1,\ldots,T10,X1,\ldots,X4,P1,P2)+\varepsilon)\\
& E(p(T1,\ldots,T10,X1,\ldots,X4,P1,P2))+E(\varepsilon)\\
COP =& p(T1,\ldots,T10,X1,\ldots,X4,P1,P2).
\end{aligned}
$$

Note that from the last equation, the experimental coefficient of performance and the polynomial $p(\cdot)$ would be equal in average. In order to know if ε has a Gaussian distribution with a zero mean and a constant variance, In Figure 6 a standardized residuals histogram by Montgomery (2001) was obtained as can be seen, the image is bell-shaped except for the three peaks to the left of the zero indicating that it does not have a perfect symmetry, to ensure that the residuals have a zero mean and constant variance. They were plotted versus coefficient of performance (COP) (see Figure 7) along with a pair of horizontal lines 3 and -3. There are points that come out of these lines, such points are called outliers, in the graph there are 81 outliers, i.e. 98.8% of the standardized residuals are within -3 to 3. Finally, it is crucial to know whether these abnormal residues affect the polynomial significantly, for this reason the 81 outliers were removed and came back to do the regression without these points and obtained a determination coefficient of $R^2 = 0.9937$. The difference is 0.0018, this result infers that outliers do not represent a significant amount, so the hypothesis, that the standardized residuals follow a Gaussian distribution with a zero mean and constant variance, is accepted.

Finally, to confirm that residues are independent, figures 7 and 8 are plotted, wherein, in fig. 8 the confidence intervals (gray lines) standardized for each residue (points in the middle) and outliers (black lines at the ends) can be observed. Both images show that the average of residues is zero (for the distribution to both sides of the axis x), the variance is constant (in the form of a gray band at the residues) and the residues are independent. This ensures the goodness of the polynomial model in Eq. (2) (see Chapter 4 and 13 from Devore (2004) for details).

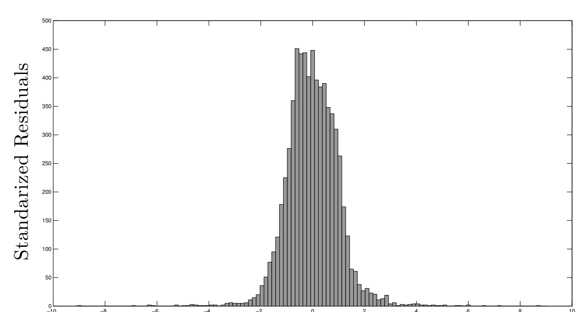

Fig. 6. Histogram of the standarized residuals.

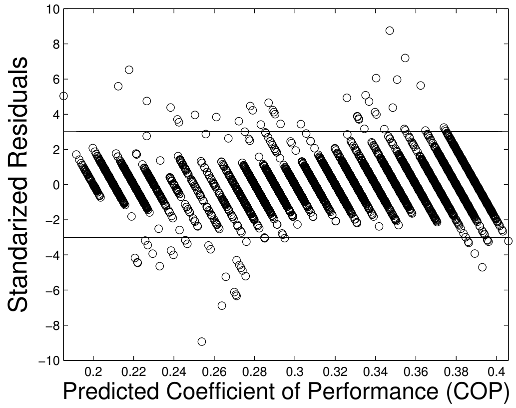

Fig. 7. Predicted coefficient of performance versus standarized residuals.

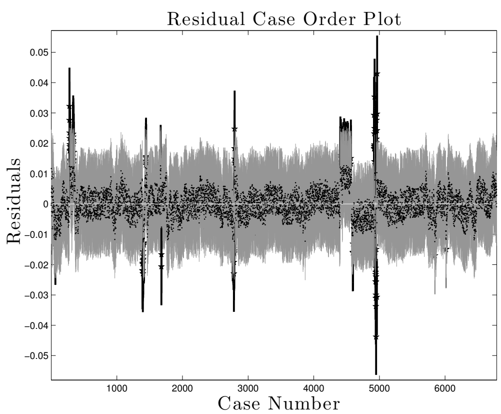

Fig. 8. Confidence intervals on the residuals with confidence level of the 95%.

Once the model is validated, it can assured that there is a linear relationship between the coefficient of performance and the monomials $T1, T3, T4$, $X3, X3^2$, $P1, P1^2, P1^3$, $P1^4, P1^5$, $P2, P2^2, P2^3$. For all the above, there is a polynomial relationship between the coefficient of performance and the variables $T1, T3, T4$, $X3, P1$ and $P2$. It is important to note that these variables are related to the absorption-desorption process.

On the other hand, the variables that have an impact on the coefficient of performance in the polynomial model are $T1, T3, T4, X3, P1$ and $P2$. Table 4 shows the contribution of each term of the polynomial model on coefficient of determination R^2. The variable with the biggest contribution to the coefficient of determination of the coefficient of performance predicted is $P1$ and the contribution is ≈ 0.5488. Another important contribution is $X3$ with a ≈ 0.3139. Therefore, the absorber pressure is the main operation variable from the point of view of the methodology, followed by the water-lithium bromide solution inlet concentration in the generator that comes from the absorber.

Table 4. The contribution of each term of the polynomial model on determination coefficient R^2

Factor	R^2
$T1$	4.2078×10^{-6}
$T3$	0.0058
$T4$	0.1738
$X3$	0.1577
$X3^2$	0.1604
$X3 + X3^2$	0.3139
$P1$	0.0869
$P1^2$	0.0916
$P1^3$	0.0948
$P1^4$	0.0965
$P1^5$	0.0968
$P1 + P1^2 + P1^3 + P1^4 + P1^5$	0.5488
$P2$	7.4473×10^{-5}
$P2^2$	6.2589×10^{-5}
$P2^3$	5.1838×10^{-5}
$P2 + P2^2 + P2^3$	0.1238

The coefficients of the polynomial model were estimated from the experimental data applying the method of least squares.

4.2 *Comparison between a polynomial model and an Artificial Neural Network(ANN) model*

The polynomial model has been carefully verified using, whenever possible, an artificial neural model reported in the open literature. Figure 9 shows a further comparison of the developed polynomial with an artificial neural model by Hernandez et al. (2009). The comparison is based on a simulated coefficient of performance versus experimental results. The determination coefficients of 0.9919 and 0.9981 were calculated for polynomial and artificial neural network models respectively. The greatest discrepancies between polynomial model and artificial neural network were observed for a coefficient of performance from 0.2 to 0.26.

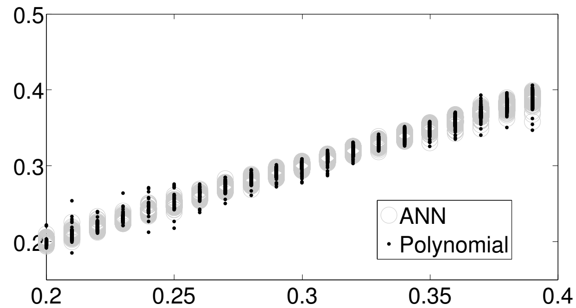

Fig. 9. Approaches to the Coeficient of Performance by an Artificial Neural Network (ANN) and multivariable polynomial (Polynomial).

It can be seen that the coefficient of performance prediction could be calculated with an artificial neural network or the polynomial methodology discussed in this work, with great confidence. It's important to note that the artificial neural network by Hernandez et al. (2009) performs COP prediction with 51 coefficients (weights and bias) and the polynomial model only with 14 coefficients. Therefore, both models can be used, at a time, to approximate the coefficient of performance.

Conclusion

A polynomial model with six inlet operation variables was successfully developed to predict coefficient of performance in a water purification process integrated to a heat transformer. The results obtained with the fit showed high accuracy with the experimental data $R^2 > 0.99$. Very high confidence level of the 95% for each coefficient of the polynomial model was verified.

This methodology can be used to simplify the complex analysis of the heat transformer with high confidence. The operation variable with the largest contribution to the determination coefficient is the absorber pressure $P1$. Consequently, greater efforts in on-line estimation, control pressure developments and equipment in a heat transformer are recommended. This methodology can be used in order to predict the performance of absorption systems. The polynomial model could be used to assess in the heat transformer technology integration in other kinds of systems, for instance, renewable energy systems or chemical industry.

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Nomenclature

COP	coefficient of performance $[-]$
P	pressure $[inHg]$
Q	heat flow $[W]$
R^2	coefficient of determination $[-]$
T	temperature $[^oC]$
X	concentration $[\%\frac{w}{w}]$
E	expected value $[-]$
Greek letters	
σ^2	standard deviation $[-]$
Subscript	
AB	absorber
CO	condenser
EV	evaporator
GE	generator

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