EXTENDED KALMAN FILTER (EKF) AND ARTIFICIAL NEURAL NETWORKS (ANN) FOR ESTIMATE OF CONCENTRATION IN A NON ISOTHERMIC CSTR OF PRODUCTION OF PROPYLENE GLYCOL

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Abstract. *The most relevant piece of equipment in the chemical industry is the chemical reactor. Those equipments usually demand high amounts of energy during its operation, and considerable costs to install and maintain. That makes necessary a decent knowledge about the operation at any time and the remote monitoring of different variables inside the reactor. Several physical sensors are present in a chemical plant, providing measurements with good precision and low sampling times, with the flow, temperature, level, and others standing out. However, when the measurement of chemical and biochemical variables is desired (e.g. biomass, average particle diameter, and product concentration) several difficulties are present, with the need for offline sampling usually being necessary. To overcome these and other difficulties the digital sensors were developed, which are mathematical models implemented in different software solutions making use of secondary physical measurements. In that sense, this study proposes the creation of soft sensors for the concentration inference in the production process of Propylene Glycol ($C_3H_8O_2$). The developed methodology was created in the following order: the mathematical modelling was initially proposed; the process was simulated in stationary and transient regimes using the software solution MATLAB – Simulink®; the soft sensors were constructed employing two different kinds of modeling, the first being a semi-empirical approach known as the extended Kalman Filter (EKF), and the second one following an empiric approach known as Artificial Neural Networks (ANN). The results obtained with the soft sensor through the artificial neural networks (CA_{ANN})-with levenberg marquardt training algorithm-presented better performance compared to CA_{EFK}, given the fact that ANN is a powerful non-linear identification algorithm and has a high capacity of generalization.The results presented were quantified using the error criteria MSE and RSME, where it was observed smaller values of estimation error for the soft sensor that used ANN.*

Keywords: *chemical reactors, soft sensor, extended Kalman filter, artificial neural network.*

1 INTRODUCTION

The growing competitiveness among the industrial, mediated by an increasingly demanding market, requires industrial plants with high quality products and lower prices. In this sense, the industry processes need to be controlled in an efficient manner, as well as operating costs. When it comes to chemical industries, the reactors are the central production equipment. So, you need to have great knowledge of such equipment, as well as its process variables and principle of operation.

On the importance of the reactors to chemical plants, the knowledge of the dynamic behavior of critical variables of operation in this process such as: temperature, concentration or composition of reactants and products, conversion, etc., becomes essential. However, when you want to implement an effective control structure, it is necessary to measure the process variable, (i.e.,concentration, in real time). What in fact to chemical or biochemical variables this measurement usually is not available. And when these real-time measurements are available, for example, using online process analyzers, your cost of maintenance and operation is quite high, in addition to demand a skilled labor for operation (CAMPOS et al., 2013).

To overcome these and other difficulties related to the estimation of variables not directly measurable in real time, it was then that arose the soft sensors (FORTUNA et al., 2005). Soft sensors (SS) are mathematical models implemented in software using measurements of secondary variables (inputs) to estimate variables of interest, this alternative arises before a

difficulty or operating cost in obtaining the desired variable (MORAIS JR., 2015). According to Kadlec et al. (2009), the construction of SS is made using two types of approaches: the phenomenological modeling and identification (black box modeling). The first is a theoretical proposition (phenomenological), which requires an understanding of the physical and chemical properties of the process. The second methodology is generated through input-output models of the process, where data are collected in plant or validated models with real data. When the two previous approaches are employed in the construction of the mathematical model, it is called gray-box modeling.

The use of black-box modeling in building SS is the possibility of recourse to facts available in plants through physical sensors. When are employees of State spaces type models, instead of the use of the term SS, used the term adaptive observers. This observer can be exact when provides the State directly, or when your tends to limit asymptotic State for infinite time (SEBORB et al., 2016). The study of the José de Assis and Maciel Filho (2000) presented a state of the art for the construction of soft sensors, with the objective of estimating the concentration in a biorretor. It is worth noting that the authors have reported the use of the extended Kalman filter (EFK) and artificial neural networks (ANN). However, they didn't make a compative between the two techniques and left a gap of how to implement real-time both techniques for reactive chemical processes.

Thus, this article proposed a methodology for constructing of two soft sensors using EKF (adaptive observers) and ANN. The methodology was implemented in a production process of propylene glycol, which occurs in a continuous stirred reactor (CSTR) operating exothermically, the model is treated as multiple input, multiple output, meaning noisy input variables are used of the process and are estimated critical variables, such as the concentration of the reactant (propylene oxide).

2 THEORETICAL FOUNDATION

The development of rigorous theoretical models may not be practical for complex processes if the model requires a large number of equations with a significant number of process variables and unknown parameters (e.g., chemical and physical properties) (SEBORG et al., 2016). An alternative approach is to develop an empirical model directly from experimental data or the application of semi-empirical methods.

In this paper modern techniques for modeling and control of robust and nonlinear chemical processes has been applied for common use, the construction of soft sensors. Thus the nonlinear modeling with the artificial neural networks has its results confronted with the semi empirical modeling through the extended kalman filter.

2.1 Extended Kalman Filter (EKF)

The Kalman Filter (KF) is an iterative mathematical procedure, which uses a set of equations and input data to estimate and predict the actual value of variables with measurement errors, or acts as an observer of States employing secondary measurements to estimate the value of difficult variables measurement (GREWAL and ANDREWS, 2001). The Extended Kalman Filter (EKF) is the non-linear version of the conventional linear KF. Given a model composed of input variables (u), (x) and (y), the algorithm of the EKF is formed by EQ (1) to (5) below.

$$\hat{x}_{k|k-1} = f\left(\hat{x}_{k-1|k-1}, u_{k-1}\right) \quad (1)$$

$$P_{k|k-1} = A_{k-1} P_{k-1|k-1} A^T{}_{K-1} + Q_k \quad (2)$$

$$K_k = P_{k|k-1} C^T{}_K \left(C P_{k|k-1} C^T{}_K + R\right)^{-1} \quad (3)$$

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k\left[y_k - h\left(\hat{x}_{k|k-1}\right)\right] \quad (4)$$

$$P_{k|k} = (I - K_k C_k) P_{k|k-1} \quad (5)$$

Where A_k and C_k are, respectively, for Jacobian matrices of the variables of state and output.

For the study, the inputs variables are: the power flow of the limiting reactant (FA_0), shirt inlet temperature (T_{a1}), feed temperature (T_0) and volumetric flow reactor inlet (v_0) and reactor temperature (T); the state variables are the temperature (T) reactor, the concentration of the limiting reactant propylene oxide (CA), excess reagent concentration (CB), product concentration propylene glycol (CC) and inert methanol concentration (C M); and the output variable (measurement) is the temperature of the reactor (T). Gaussian noise was inserted with zero mean and covariance equal to 0.1 in the input variables and also was added a covariance equal to 0.01 in the measurement of temperature.

2.2 Artificial Neural Networks (ANN)

Artificial neural networks (ANN) are an important class of empirical nonlinear models. The exceptional computational abilities of the human brain have motivated the concept of an ANN. The brain can perform certain types of computation, such as perception, pattern recognition, and motor control, much faster than existing digital computers (HAYKIN, 2009; HAGAN et al., 2014).

A multilayer feed-forward ANN was utilised in this study. Multilayer Perceptron networks (MLP) are known for their wide range of application in several problems from different knowledge areas and are also considered one of the ANN most versatile architectures regarding applicability (SILVA et al., 2017). Among these potential areas for chemical enginering, the most important is the process identification and control. This type of network contains a layer of input neurons which are interconnected to the nodes in one or more hidden layers which are linked in turn to the nodes in the output layer see Fig. 1. This type of ANN is trained by using inputs and the corresponding output data derived from the secundary measurements, in this reseach provided through the mathematical model of the reactor.

In the forward phase, the input values x_1, x_2, ... x_N are fed through the network and during transmission are modified by the weighting fixed and transfer function (sigmoid logarithm and sigmoid tangent transfer functions were tested in the present study), these are propagated through the network, layer by layer, until it reaches the outputs (y). In the backward phase, an error signal is produced by comparing the y returned by the network with the y desired. The eventual predicted values, which are fed into the output nodes, are compared with the corresponding measured results and any differences, i.e. the ‘‘errors”, are propagated back through the network and used to adjust the weightings of the connections. This process is known as single training cycle or iteration.

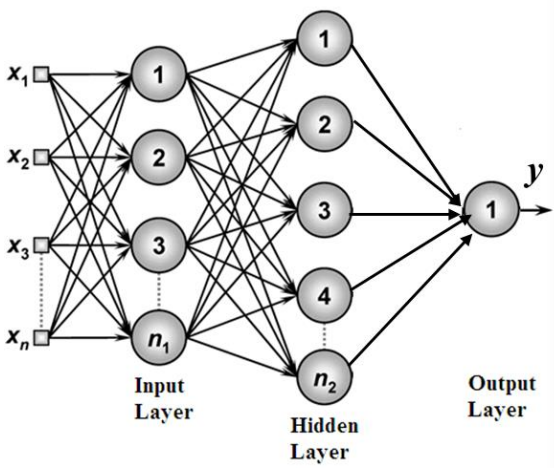

Figure 1. Schematic representation of a MLP ANN.

The development of the back-propagation algorithm in the mid-1980s presented a computationally efficient method for the training of multilayer perceptrons. However, the backpropagation algorithm has a slow convergence process, so alternative methods have been developed to obtain higher convergence speed (HAGAN et al., 2014).

The Levenberg-Maquardt training algorithm is an iterative method consisting of an improvement of the Gauss-Newton method (LEVENBERG, 1994). Given a starting point x0, a series of vectors x1, x2, ..., xn is produced until it converges to a local minimum x*, for which the function must be adjusted. Such algorithm needs to store a square matrix with dimension in the order of the number of connections, so it is important to use a network with fewer than a hundred connections.

Consider F(w) which is a second order function in terms of the weight vector w, its gradient vector and H its Hessian matrix. According to the Levenberg Maquardt algorithm, the ideal fit Δw applied to the parameter vector is provided through Eq. (6).

$$\Delta \mathrm{w} = \mathrm{w}_{\mathrm{K+1}} - \mathrm{w}_{\mathrm{K}} = \left[\mathrm{H} + \mu\, \mathrm{I}\right]^{-1} g \tag{6}$$

where I is the identity matrix of the same dimensions as H and μ is a regularizing, or loading, parameter that forces the sum matrix (H+μI) to be positive definite and safely well conditioned throughout the computation.

The nature of the complexity of Hessian H (w) represents a computational limitation, its better representative form and with a smaller computational effort can be expressed through Eq. (7), the desired adjustment calculated for each iteration of the Levenberg Maquardt algorithm with the cost function ξfc(w).

$$H(w) \approx \frac{\partial^2 \xi_{fc}(w)}{\partial w^2} = \frac{1}{N} \sum_{i=1}^{N} \left[\frac{\partial F(x(i);w)}{\partial w} \right] \left[\frac{\partial F(x(i);w)}{\partial w} \right]^T \tag{7}$$

The use of the Equation (8) as approximation is justified when the Levenberg algorithm is operating in the neighborhood of a local or global minimum (x^*).

During the training of the Levenberg Maquardt algorithm and other training algorithms there are difficulties in establishing the ideal stopping point (an overall minimum value) because the training error starts with a high value that decreases rapidly and continues to decrease slowly, tending to reach a local minimum on the error surface. It is important to note that ANN can be used as a tool for evaluating ANNs, and it can be used to determine whether the ANN training should be terminated. In this study the Early-Stopping Method was adopted using cross-validation, which interrogates the training at each C epochs (cycles) and an estimation of the network error is performed based on a set of data.

3 METHODOLOGY

It was initially developed the mathematical modeling of the reactor for the production of propylene glycol. Shortly thereafter, the process was simulated using the software Matlab-Simulink®, being inserted some disorders for transient behavior analysis of the process. Subsequently, the EKF algorithms have been implemented and the ANN in order to estimate critical variables of the process. Being employee error criteria to assess the estimate.

3.1 Chemical process studied

In the process, the propylene glycol is produced in a reactor CSTR, according to Fig. 2. In the propylene oxide is hydrolyzed, the methanol used as inert and sulfuric acid as a catalyst.

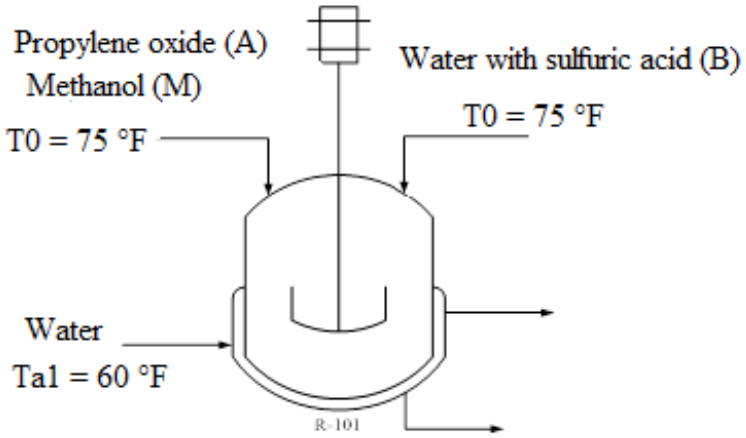

Figure 2. Production of propylene glycol.

The Equation (8) represents the chemical reaction involved in the production process of propylene glycol.

$$C_3OH_6 + H_2O \xrightarrow{H_2SO_4} C_CO_2H_6 \tag{8}$$

To facilitate the writing of equations of mass and energy balance the compounds involved in the reaction above are referred to as: A consists of propylene oxide (reagent), B is the water (reagent), C is the propylene glycol (product) and M is methanol (inert). The law of speed of reaction is given by Eq. (9).

$$-r_A = k * C_A \tag{9}$$

Being CA concentration of propylene oxide and k rate constant.

It is known by the stoichiometry of the reaction that the relationship of Eq. (10) is true.

$$-r_A = -r_B = r_C \tag{10}$$

3.2 Mathematical modelling of the process

The purpose of modeling is to determine a set of mathematical equations (algebraic, differential and integral) describe the behavior of the process when are modified parameters and/or variables of this.

Material balances have been developed in terms of molar concentration for each component in the reactor, Eq. (11) to (14).

For A:

$$\frac{dCA}{dt} = r_A + \left(\frac{CA_0 - CA}{V}\right) * v_0 \tag{11}$$

For B:

$$\frac{dCB}{dt} = r_B + \left(\frac{CB_0 - CB}{V}\right) * v_0 \tag{12}$$

For C:

$$\frac{dCC}{dt} = r_C + \left(\frac{0 - CC}{V}\right) * v_0 \tag{13}$$

For M:

$$\frac{dCM}{dt} = \left(\frac{CM_0 - CM}{V}\right) * v_0 \tag{14}$$

Where: CA_0 and CA are, respectively, the concentrations of propylene oxide in the inlet and outlet streams of the reactor; CB_0 and CB correspond, respectively, the concentration of water in the inlet and outlet streams of the reactor; CM_0 and CM correspond respectively, methanol concentrations in the inlet and outlet streams of the reactor; CC is the concentration of the product propylene glycol in the reactor output; r_A, r_B and r_C are, respectively, the rates of reaction of compound A, B and C; and V and v_0 are, respectively, the volume and the volumetric flow of reactor feed stream.

The balance of enegy in the reactor provides the Eq. (15).

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W} + F_{A0} * \theta Cp * (T - T_o) - \Delta H * - r_A * V}{NCp} \tag{15}$$

Where: Q is the heat removed; W is the work; ϴCp is the sum of the product of the molar specific heat ratio of each component; T and T_0 are, respectively, the temperature of the output and input streams of the reactor; ΔH is the change of enthalpy in reaction; and NCp is the sum of the product between the number of moles and the enthalpy of ach component. The parameters and initial conditions are shown in Table 1.

Table 1. Parameters and operating conditions of CSTR reactor*.

Parameters and operating conditions	**Values and units**
V	66,8092 [ft³]
UA	16000 [Btu/h.°F]
T_{a1}	60 [° F]
T_0	75 [° F]
FA_0	80 [lbmol/h]
magua	1000 [lbmol/h]
ΔH	-36000 [Btu/lbmol]
ϴCp	284,375 [Btu/lbmol.°F]
R	1,987 [Btu/lbmol.°R]
v_0	441,4640 [ft³/h]
τ	0,1514 [h^{-1}]
CA_0	0,1812 [lbmol/ft³]
CB_0	2,2652 [lbmol/ft³]
CM_0	0,2265 [lbmol/ft³]
cpA	35 [Btu/lbmol.°F]
cpB	18 [Btu/lbmol.°F]
cpC	46 [Btu/lbmol.°F]
cpM	19,5 [Btu/lbmol.°F]
CAi	0 [lbmol/ft³]
CBi	3,45 [lbmol/ft³]
CCi	0 [lbmol/ft³]
CMi	0 [lbmol/ft³]
Ti	75 [° F]

* The data were obtained in Furusawa et al. (1969) and Fogler (2009).

As previously mentioned, the term observer of state is given the type of model applied in the construction of soft sensors with ANN and EKF.

4 RESULTS AND DISCUSSION

4.1 Analysis of the process dynamics

In order to evaluate the transient behavior of the process were resolved the set of 5 (five) ordinary coupled equations, presented in section 3.2, in software Matlab-Simulink®. The graphics of the Fig. 3 a), b), c), d) and e) are, respectively, the transient behavior of the concentrations of CA, CB, CC and CM and T during a 10-hour simulation time.

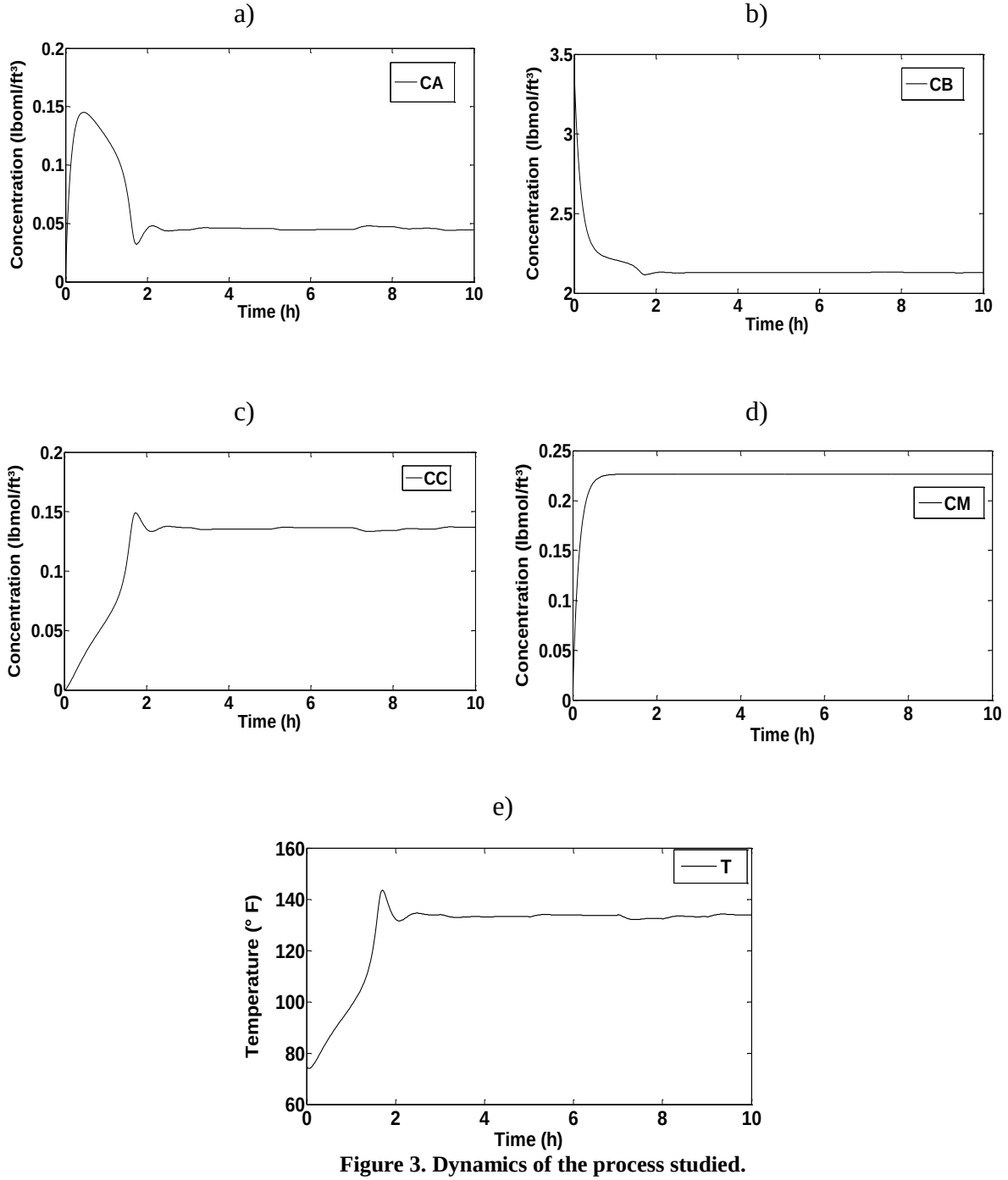

Figure 3. Dynamics of the process studied.

According to the Fig. 3 a), there is an increase in the concentration of the limiting reactant (A) until the time of 0.25 h, soon after its reduction occurs, caused by its use during the beginning of the reaction. Thus, an increase in the concentration of the product until the time of 1.8 hours, as the graph of Fig. 3 d). Was evaluated also the conversion of the process overtime according to Fig. 4.

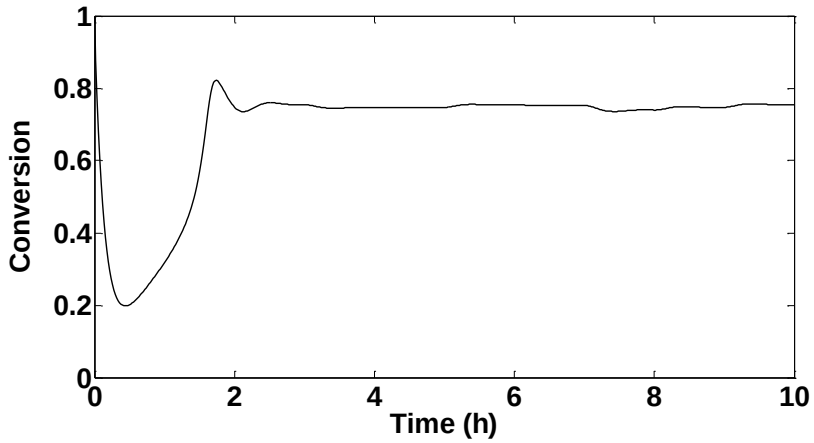

Figure 4. Conversion over time.

Based on the graph of Fig. 4, the conversion initially decreases due to increased concentration of propylene oxide in the reactor. However, when the reaction actually begins to happen is a significant increase in conversion because the largest reagent consumption. As the process reaches the stationary regime around 1.8 hours, from that moment, the conversion remains constant.

4.2 Data Collection for Offline Training

For the offline training of the neural networks were made perturbations of ± 5%, ± 10% and ± 15% in the steady state value in that following process variables: FA_0 , T_0, v_0, T_{a1}. Theses pertubations were made with the objective of moving the process to different operating conditions. The graphs of Figures 5 a), b), c) and d) show the transient behavior of feed molar flow, feed temperature, feed molar flow and the jacket temperature of the propylene glycol production reactor . The transient effect of the perturbations carried out in the graphs of Fig. 5 had as sole and exclusive objective to place the concentrations and the conversion of the propylene glycol production reactor at levels in which the inference models, artificial neural networks and extended kalman filter are capable of estimating. A total of 1002 data were collected during 50 hours of simulation, with a sample time of 0.05 h.

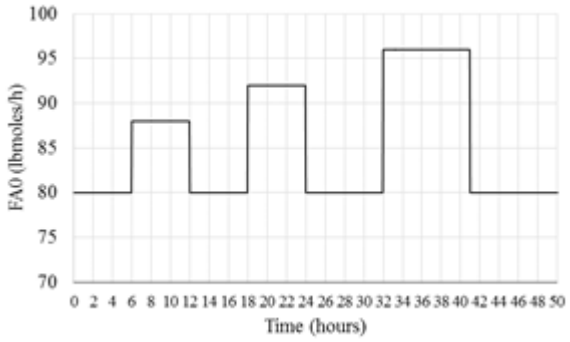

Figure 5. a). Steps in molar flow rate.

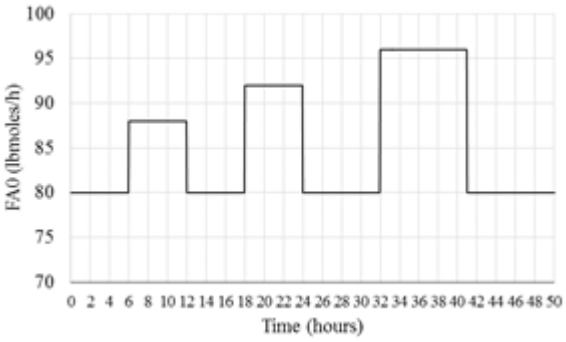

Figure 5. b). Steps in temperature feed.

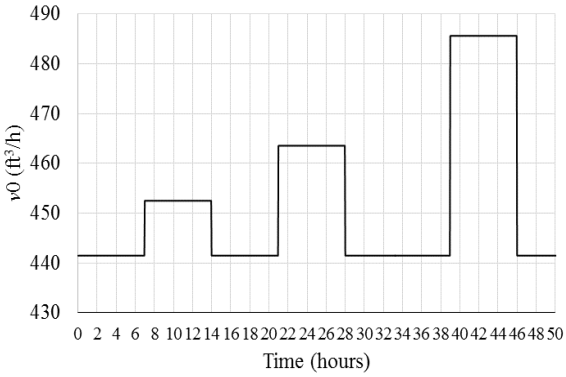

Figure 5. c). Steps in molar volumetric flow rate.

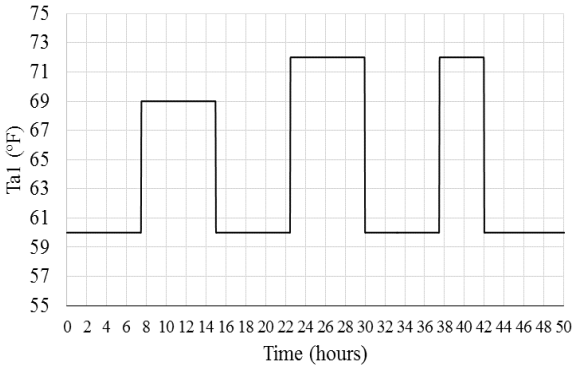

Figure 5. d). Steps in coolant temperature.

4.3 Results of Soft Sensor with ANN Offline

The training algorithm chosen was Levenberg-Marquardt (LVM), which, among other training algorithms, has a faster convergence. After all the tests to evaluate the choice of the architecture, the activation function, the training algorithm and the number of layers with their respective number of neurons, about 120 RNAs were trained. The activation function used was the logsig for presenting a balance between linear and nonlinear performance. Since the logsig function has a normalization interval [0 1], the input signals were normalized for better inference performance since the inputs had different units. In addition, in the process of ANN learning, it is customary to divide the data between the training, validation and test steps. In this study, 70% of the data set were used for the training, 15% for the validation and 15% for the test.

The best result is presented here, that is, the smallest error between the actual data and the estimated propylene oxide (reagent) concentration (CA) in the reactor outlet stream, was obtained with the ANN topology [15 10 15]: one input layer (with 15 neurons) and two hidden layers (with 10 and 15 neurons each, respectively), as shown in Table 2 below.

Table 2. ANN data with best offline result for composition inference.

Topology	[15 10 15]
Training Algorithm	Levenberg-Maquardt
Architecture	Multilayer perceptron
Activation function	Logsig
Error performance	2,10 x 10^{-6}
Number of iterations	54

Generally, regression analysis of the data is used to evaluate the relationship between two or more variables. It is a technique that allows visualizing the relation of a dependent variable to other independent variables (MONTGOMERY and RUNGE, 2014). Thus, the adjustment of the data in the training, validation and test steps for this chosen neural network is shown in Fig. 6 a) e b).

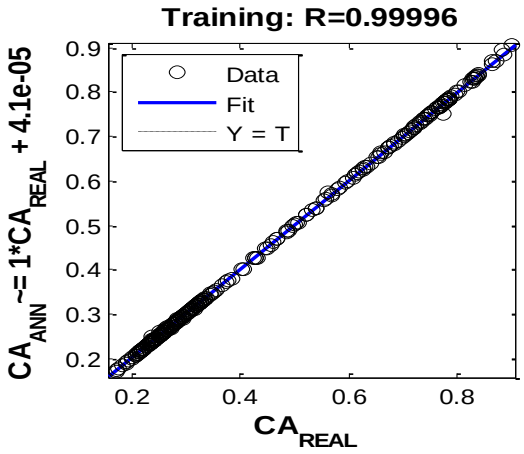

Figure. 6. a) Regression with training data.

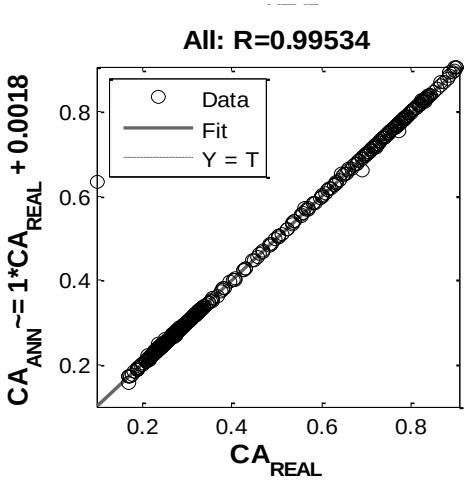

Figure. 6. a) Regression with all data.

As can be seen in the graphs above, the estimates generated by the neural network model fit with the real data at a 45º slope, which provides a fitting conclusion to fit the experimental data. The graphs of Figures 7 a) and b), respectively, present the results of the CA(t) soft sensor neural training and all data set versus simulation time, respectively, compared to data from the matemathical modeling-Real (simulation in the Matlab® software).

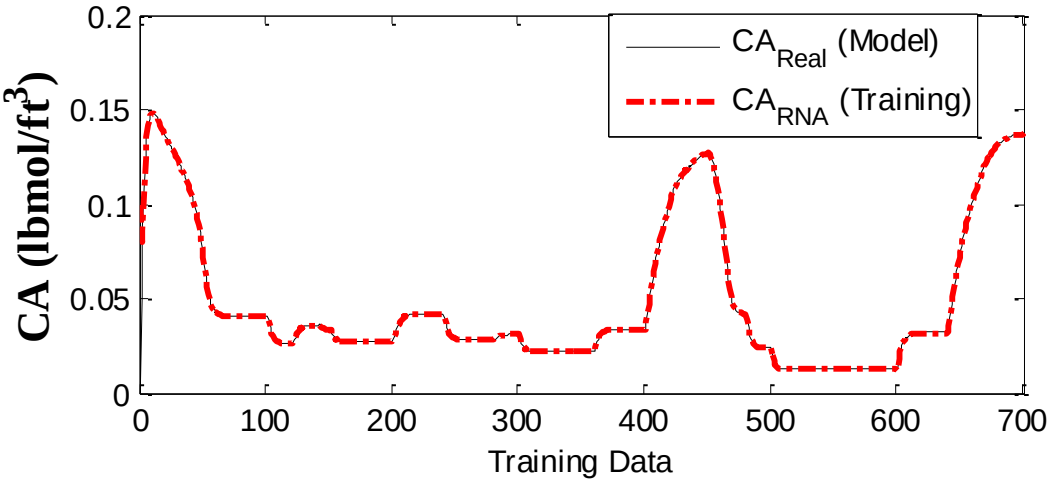

Figure 7. a) Soft sensor with ANN, training data set.

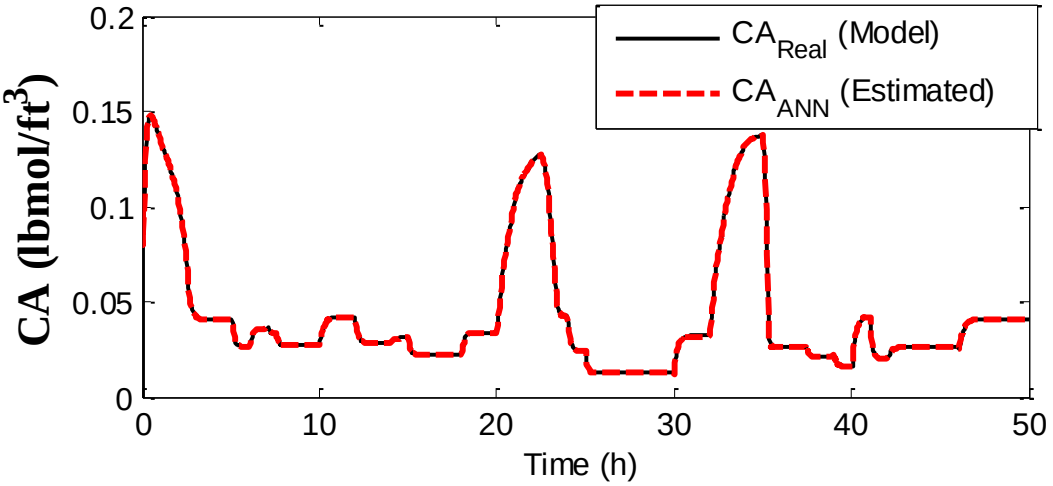

Figure 7. a) Soft sensor with ANN, all data set.

It's verified that the ANN soft sensor presented good results for inference, According to the Fig 7, of the concentration of the reagent from the second distillation tower. It is important to observe the occurrence of several perturbations in the input variables, displacing the process variable under different transient operating conditions, which increases the robustness of the ANN soft sensor and provides a good reliability of estimation.

4.4 Results of Soft Sensor with using the EKF

The noise and the measurement process were considered as gaussian noises of zero mean and variance 0.01 and 0.02, respectively.The graph of Fig. 8 shows the actual concentration of propylene oxide (limiting reactant) in comparison with the soft sensor inference using EKF. As you can see the concentration value estimated by the EKF, though showing the same profile on the chart, presented certain discrepancy in comparison to the value of the process.

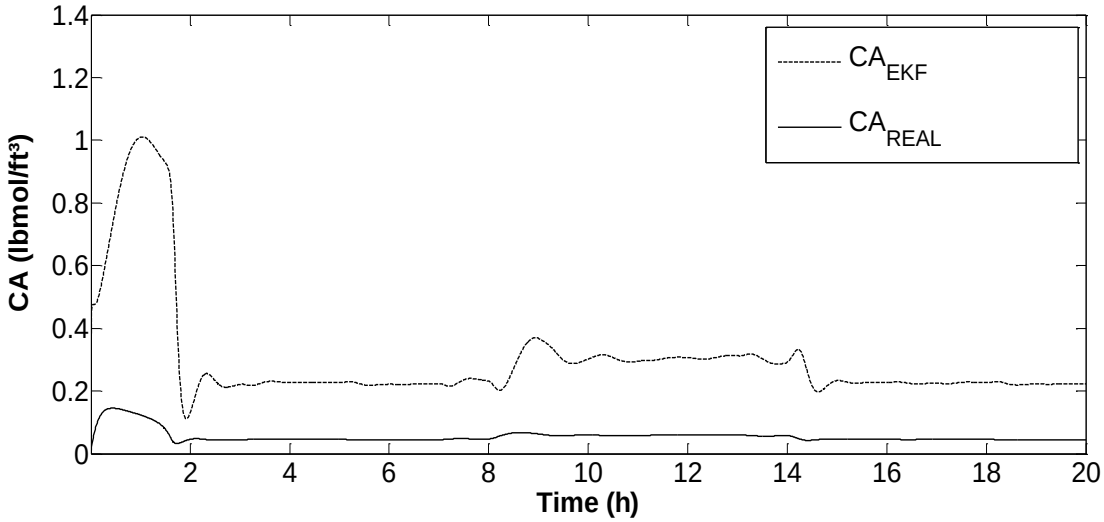

Figure 8. Estimation of the cocnentration by the FKE.

The quantification of the error in the estimation of the concentration of propylene oxide. The discrepancy between the estimated and actual values can be related with the tuning parameters of the Kalman filter.

4.5 Online Transient Estimation of the Concentration

The results presented in this section are derived from the transient simulation of the process. In this case, the MLP neural network with configuration [15 10 15] and the extended Kalman filter provided the concentration in real time (online), respectively presented in the graph of Fig. 9 by CA_{ANN} and CA_{EFK}, as compared to the model of the process (CAREAL).

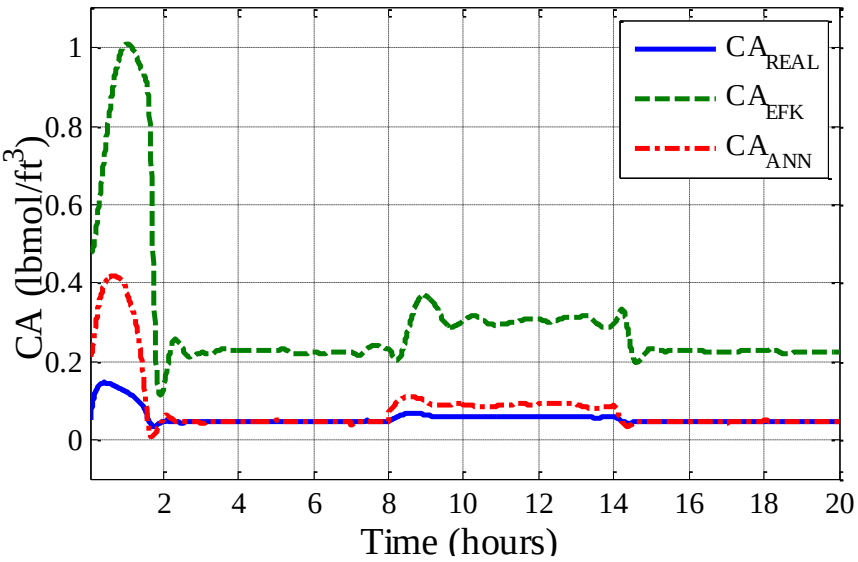

Figure 9. Comparison of the concentration provided by the sensor with ANN and EFK versus process model (Real).

In the graph of Fig. 9, disturbances of +20 (at time of 8 hours) and -20% (at time point of 14 hours) were performed, both in the molar flow rate (FA_0). It can be seen from the same graph that the ANN estimation (CA_{ANN}) is able to be closer to the actual process concentration (CA_{REAL}) compared to the inference provided by the soft sensor with EFK (CA_{EFK}). It's important to mention that after the second disturbance in FA_0 the concentrations inferenced by both soft sensors returned to the steady state of operation.

The uncertainties brought in by observation errors or the method used to compare model and observations are considered here. In order to make a quantitative analysis the Mean square error (MSE) and the Root mean square error (RMSE) are calculated for the data set online, provided by Eq. (16) and (17), respectively.

$$MSE = \sum_{i=1}^{N} \frac{1}{N}(y - \hat{y})^2 \tag{16}$$

$$RMSE = \sqrt{\sum_{i=1}^{N} \frac{1}{N}(y - \hat{y})^2} \tag{17}$$

Where N is the total number of samples during the whole simulation; y is the actual concentration given by the mathematical model of the process; and $\hat{y}$ is the concentration estimated by the soft sensors.

Table 3 shows the MSE and RMSE values for the reagent concentration in the output stream of the propylene glycol production reactor.

Table 3. Estimate error parameters.

SOFT SENSOR	MSE	RMSE
CA_{EKF}	9.07×10^{-2}	0.30112
CA_{ANN}	4.3×10^{-3}	0.06549

5 CONCLUSIONS

In this study aimed to develop a methodology for the construction of two soft sensors using two distinct identification techniques for nonlinear processes: black-box modeling (with ANN) and semi-empirical modeling (with EFK). Both the soft sensor with ANN and the soft sensor with EFK had flow rate FA_0 and v_0 inputs and temperatures T_0, T_{a1} and T. Neural network training was performed with multilayer networks, with the best network topology defined through of the error minimization parameters. With this, an ANN was chosen to estimate robust online concentration to the point of overcoming characteristic disturbances of the process. Thus, an ANN was defined with 3 hidden layers, a simulation logarithmic activation function, with the Levenberg Maquardt training algorithm and a stop criterion through cross validation. The data for offline training of the ANN were collected through the transient simulation of the CSTR reactor for the production of propylene glycol, the concentration of the reagent in the process output stream was the variable to be estimated. For inference through the soft sensor with EFK

were calculations of Jacobian matrices of the variables of state and output. Gaussian noises was inserted with zero mean and covariance equal to 0.1 in the input variables and also was added a covariance equal to 0.01 in the measurement of temperature. The results showed that the accentuated concentration curve at the beginning of the process proves to be a difficult monitoring point due to the large changes in temperature and concentrations inherent in exothermic reactions.Thus, it was found that the estimation using the extended kalman filter (CA_{EFK}) presented difficulties in approaching the actual concentration of the process. In fact, this problem can be attributed to the difficulty of adjusting parameters correlated to kalman gain, such as the process variance matrix (Q) and the covariance matrix of the estimation (P). It's worth mentioning that for future work, a study on the tuning of these parameters can be inserted.The results obtained with the soft sensor through the artificial neural networks (CA_{ANN})-with levenberg marquardt training algorithm-presented better performance compared to CA_{EFK}, given the fact that ANN is a powerful non-linear identification algorithm and has a high capacity of generalization.The results presented were quantified using the error criteria MSE and RSME, where it was observed smaller values of estimation error for the soft sensor that used ANN.

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