Soft Sensor based on Adaptive Linear Network for Distillation Process

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ABSTRACT
The main objective in refining units is to keep the product quality within specifications in the faces of disturbances. Online measurements of product composition using composition analyser are neither easy nor economically viable. In an effort to overcome these difficulties various soft sensors are designed in the recent years. In this research work, the authors have proposed the design of neural network based soft sensor for two types of chemical processes i.e. reactive distillation process and multicomponent distillation process. The designed soft sensor is based on adaptive linear network, Adaline and is used to infer the product composition from the temperature profile of the respective processes. For a comparative study Levenberg Marquardt based artificial neural network soft sensor is also designed. It is observed from the results that the Adaline based soft sensor is more efficient in comparison to LM based ANN soft sensor in terms of accuracy, time taken for training and memory usage.

General Terms
Application of Adaptive Linear Network in distillation process.

Keywords
Adaline soft sensor, LM soft sensor, Reactive distillation process, Multicomponent distillation.

1. INTRODUCTION
For successful control of distillation process, the online measurement of product composition is quite important. The measurements using composition analysers are difficult because they are expensive, difficult to maintain, require frequent calibration and have undesirable time delays. Therefore to avoid such type of difficulties, the composition is predicted from secondary measurements such as temperature measurements, pressure, heat input, reflux flow etc. [1][2]. Sungyong Park and Chaonghun Han [3] proposed a design methodology to design a soft sensor for chemical processes that can handle the correlations among many process variables and nonlinearities based on smoothness concepts. Yao Wu and Xionglin Luo [4] introduced multirate data fusion technology based on Kalman filter into soft sensor maintenance, to integrate the soft sensor model estimation with process measurement. The results demonstrated that the multirate Kalman filter approach provides improved accuracy and reliability of soft estimation when essentially dynamics is included in the Kalman filtering model and the filter parameters are properly tuned. Pierantonio Facco *et al*. [5] developed a moving average partial least square soft sensor for online product quality estimation in an industrial batch polymerization process. Almila Bahar and Canan Ozgen [6] designed an ANN based estimator system and used it in the feedback inferential control algorithm. Inputs to the controller are estimated compositions from ANN and the reflux ratio information. In the control law scheduling policy is used and predefined set points are the optimal reflux ratio profile. A. Rogina *et al*. [7] conducted multiple linear regression analysis and used neural networks based models to develop soft sensors. The best results were obtained with multilayer perceptron and radial basis function neural networks on considering statistical and sensitivity analysis. Ming-Da Ma *et al*. [8] developed an adaptive soft sensor based on statistical identification of key variables. The inferential model built by the selected key variables predicted accurately and matched the real plant situation which made it useful for industrial applications. S.R. Vijaya Raghavan *et al*. [9] presented the design and implementation of a recurrent neural network (RNN) based inferential state estimation scheme for an ideal reactive distillation column. The performance of RNN shows better state estimation capability as compared to other state estimation schemes in terms of qualitative and quantitative performance indices. L. Fortuna *et al.* [10] designed neural based soft sensors to improve product quality monitoring and control in a refinery by estimating the stabilized gasoline concentration in the top flow and the butane concentration in the bottom flow of a debutanizer column, on the basis of a set of available measurements. Fatima Barcelo-Rico *et al.* [11] presented a methodology for the design of a fuzzy controller applicable to continuous process based on local fuzzy models and velocity linearization.

The present work deals with the design of two types of artificial neural network based soft sensors. The adaptive linear network is used to estimate the product composition of two distillation processes from the respective temperature profiles. The LM soft sensor based on Levenberg-Marquardt trained artificial neural network is also designed for comparison purpose [2]. The proposed sensors are discussed in the next section.

2. PROPOSED SOFT SENSORS

2.1 Adaptive Linear Network (Adaline) Soft Sensor
Adaptive Linear Network (Adaline) developed by Widrow and Hoff is found to use bipolar activation functions for both the input signals and target output (1960) [12]. The architecture of an Adaline is shown in Fig. 1. The Adaline has only one output unit which receives input from several units and also from bias whose action is always +1. The Adaline resembles a single layer

network. In Fig. 1 an input layer with $x_1,...,x_n$ and bias and an output layer with only one output neuron is present. The input and output neurons possess weighted interconnections.

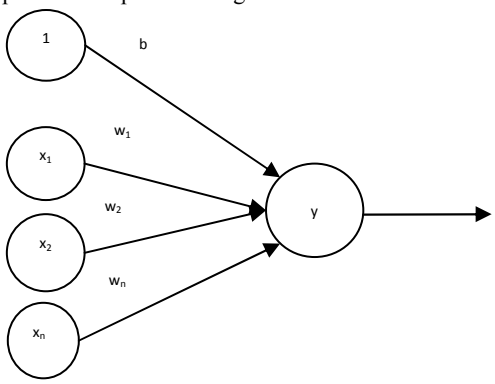


Fig. 1 Architecture of an Adaline

The output *y* of the Adaline is given as,

$$y = \sum_{i=1}^{n} w_i x_i + b \tag{1}$$

The weights are trained using least mean square algorithm based on the use of [13] instantaneous values of cost function namely,

$$E(\boldsymbol{w}) = \frac{1}{2} e^2(n) \tag{2}$$

where *e(n)* is the error signal measured at time n. Differentiating *E(w)* with respect to the weight vector ***w*** yield

$$\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = e(n) \frac{\partial e(n)}{\partial \boldsymbol{w}} \tag{3}$$

The algorithm operates with a linear neuron so the error signal is expressed as

$$e(n) = d(n) - \boldsymbol{x}^T(n)\boldsymbol{w}(n) \tag{4}$$

hence

$$\frac{\partial e(n)}{\partial \boldsymbol{w}(n)} = -\boldsymbol{x}(n) \tag{5}$$

and

$$\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}(n)} = -\boldsymbol{x}(n) e(n) \tag{6}$$

using the later result as an estimate of gradient vector

$$\hat{\boldsymbol{g}}(n) = -\boldsymbol{x}(n) e(n) \tag{7}$$

Finally using the eqn. (7) for the gradient vector in equation of weight upgradation for the method of steepest descent, the least mean square algorithm is formulated as

$$\hat{\boldsymbol{w}}(n+1) = \hat{\boldsymbol{w}}(n) + \eta \boldsymbol{x}(n) e(n) \tag{8}$$

where, η is the learning rate parameter.

In this paper single layer Adaline network is used to predict the composition of distillate product from temperature profile of the column.

2.2 Levenberg-Marquardt Soft Sensor

The Levenberg-Marquardt soft sensor is an LM trained artificial neural network. The algorithm minimizes the functions that are sums of squares of other nonlinear functions [14]. The neural network training uses mean square error as the performance index which can be minimized using LM algorithm.

In present work the Levenberg-Marquardt algorithm is applied to estimate the composition of multicomponent distillation process and reactive distillation process [7]. If each target occurs with equal probability, the mean squared error is proportional to the sum of squared error over the Q targets in the training set.

$$F(x) = \sum_{q=1}^{Q} \left(t_q - a_q\right)^T (t_q - a_q)$$

$$= \sum_{q=1}^{Q} {e_q}^T e_q = \sum_{q=1}^{Q} \sum_{j=1}^{s^M} (e_{j,q})^2 = \sum_{i=1}^{N} (v_i)^2 \tag{9}$$

where $e_{j,q}$ is the jth element of the error for the qth input /target pair.

The key step in the Levenberg-Marquardt algorithm is the computation of the Jacobian matrix. To perform this computation, a variation of back propagation algorithm is used. To create the Jacobian matrix, the computation of derivatives of the errors is needed, instead of the derivatives of the squared errors. Note that the error vector is

$$V^T = [v_1\, v_2, \dots, v_N] = [e_{11}\, e_{21}, \dots, e_{s^M,1}.\, e_{12}, \dots, e_{s^M,Q}] \tag{10}$$

The parameter vector is

$$X^T = [x_1\, x_2, \dots, x_N] = [w_{11}^1 w_{12}^1, \dots, w_{s^1,R}, b_1^1, \dots, b_{s^1}^1, w_{11}^2, \dots,\, b_{s^M}^M] \tag{11}$$

The standard back propagation method calculates terms like

$$\frac{\partial F}{\partial x_l} = \frac{\partial e_q^T e_q}{\partial x_l} \tag{12}$$

For the elements of the Jacobian matrix that are needed for the Levenberg-Marquardt algorithm need to calculate terms like

$$[\boldsymbol{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial x_l} \tag{13}$$

Now the elements of Jacobian matrix can be computed as

$$[\boldsymbol{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial w_{i,j}^m} = \frac{\partial e_{k,q}}{\partial n_{i,q}^m} \times \frac{\partial n_{i,q}^m}{\partial w_{i,j}^m} = \tilde{s}_{i,h}^m \times \frac{\partial n_{i,q}^m}{\partial w_{i,j}^m} = \tilde{s}_{i,h}^m \times a_{j,q}^{m-1} \tag{14}$$

or if x_l is a bias

$$\left(n_i^m = \sum_{j=1}^{s^{m-1}} w_{i,j}^m a_j^{m-1} + b_i^m, Therefore \quad \frac{\partial n_i^m}{\partial w_{i,j}^m} = a_j^{m-1}\right)$$

and $\left(\frac{\partial n_i^m}{\partial b_i^m} = 1\right)$

$$[\boldsymbol{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial b_i^m} = \frac{\partial e_{k,q}}{\partial n_{i,q}^m} \times \frac{\partial n_{i,q}^m}{\partial b_i^m} = \tilde{s}_{i,h}^m \times \frac{\partial n_{i,q}^m}{\partial b_i^m} = \tilde{s}_{i,h}^m \tag{15}$$

The Marquardt sensitivities can be computed through the same recurrence relations as the standard sensitivities (eq. 16), with one modification at the final layer. For the Marquardt sensitivities at the final layer we have

$$\tilde{s}_{i,h}^M = \frac{\partial v_h}{\partial n_{i,q}^M} = \frac{\partial e_{k,q}}{\partial n_{i,q}^M} = \frac{\partial \left(t_{k,q} - a_{k,q}^M\right)}{\partial n_{i,q}^M} = -\frac{\partial a_{k,q}^M}{\partial n_{k,q}^M}$$

$$= \begin{cases} -\dot{f}^M(n_{i,q}^M) \; for \; i = k \\ 0 \qquad for \; i \neq k \end{cases} \tag{16}$$

Therefore when the input p_q are applied to the network and the corresponding network output a_q^M are calculated, the Levenberg-Marquardt back propagation is initialized with

$$\tilde{s}_q^M = -\dot{F}^M(n_q^M) \tag{17}$$

where $\dot{F}^M(n_q^M)$ is defined in equation (17). Each column of the matrix $\tilde{s}_q^M$ must be back propagated through the network using equation (16) to produce one row of the Jacobian matrix. The column can also be back propagated together using

$$\tilde{s}_q^m = -\dot{F}^m(n_q^m)(w^{m+1})^T \tilde{s}_q^{m+1} \tag{18}$$

The total Marquardt sensitivity matrices for each layer are then created by augmenting the matrices computed for each input:

$$\tilde{\boldsymbol{s}}^M = [\tilde{s}_1^m, \quad \tilde{s}_2^m, \dots, \quad \tilde{s}_q^m] \tag{19}$$

It is to be noted that for each input presented to the network the sensitivity vectors $\tilde{\boldsymbol{s}}^M$ will be back propagated. This is because the derivative of each individual error is computed, rather than the derivative of the sum of squares of the errors. For every input applied to the network there will be $\tilde{\boldsymbol{s}}^M$ errors (one for each element of the network output).

The Levenberg-Marquardt technique derived in above section is summarized in the following steps.

Step1: Compute the error using target and actual output calculated by network. Compute the sum of squared errors for over all outputs using equation (9).

Step2: The Jacobian matrix is calculated using error with respective inputs.

Step3: The sensitivities are calculated with the recurrence relations in equation (17) initializing with the equation (16).

Step4: The individual matrices are augmented into the Marquardt sensitivities using equation (19) and compute the elements of the Jacobian matrix using equations (14) and (15).

Step5: Solve the following equation to get the value of Δx_k.

$$\Delta x_k = -[\boldsymbol{J}^T(x_k)\boldsymbol{J}(x_k) + \mu_k \boldsymbol{I}]^{-1}\boldsymbol{J}^T(x_k)\boldsymbol{v}(x_k) \tag{20}$$

Step6: Recompute the sum of squared errors using the new value $x_k + \Delta x_k$. If the new sum of squares of errors is smaller than the error computed in step 1 then divide μ by ϑ and let $x_{k+1} = x_k + \Delta x_k$ and go back to step 1. If the sum of squares is not reduced then multiply μ by ϑ, and go back to step 3.

The LM algorithm discussed above is used to update the weights of the artificial neural network and the network is then used for estimating the distillate composition.

3. CASE STUDIES

Two cases of applications to distillation column are analysed; reactive distillation process and Multi component distillation process. The proposed soft sensors are used to estimate the product composition for the two processes.

3.1 Reactive Distillation Process

Reactive distillation is a process of chemical reaction and separation of the products in the common chamber. It is a highly nonlinear and complex process. The chemical industry prefers reactive distillation due to its high gain and compact nature. Reactive Distillation Column (RDC) is an ideal two-reactant-two-product column proposed by Al-Arfaj and Luyben [15] and later developed into state space model. It consists of a reactive section in the middle and non-reactive rectifying and stripping sections at the top and bottom respectively.

The column consists of Reactive Trays (NRX=9) in the middle, Rectifying Trays (NR=5) in the top and Stripping Trays (NS=5) in the bottom. The trays of the column are numbered from reboiler to condenser. The reaction that takes place in the reactive zone is exothermic liquid-vapour in nature and is given by

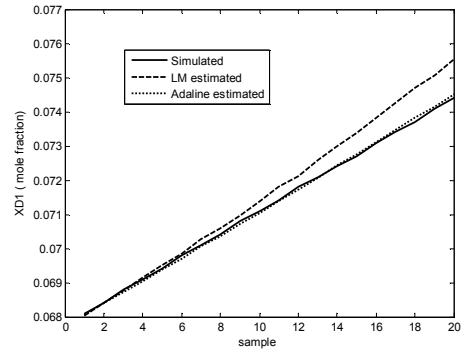
$$A + B \leftrightarrow C + D \tag{21}$$

During the distillation process, the reactant B which is one of the input feeds is recovered in the rectifying section from the output product C whereas the second feed i.e. reactant A, is recovered from output product D in the stripping section. The reactive section comprises the middle section of the reactive distillation column where the reactants A and B react to produce C and D. The reaction generates the heat which is then used for the distillation of the products. The products are separated to prevent any undesired reaction between reactants A and B and products C and D. The volatilities of the products and reactants are such that

$$\alpha_c > \alpha_a > \alpha_b > \alpha_d \tag{22}$$

where α_j is the volatility of the jth component, $j = a, b, c, d$.

The mathematical model of reactive distillation column is simulated in MATLAB. The training and testing data for soft sensors is generated by simulating the model for variable feed flow rates. The corresponding changes in the temperature profile and distillate composition are then considered for training as well as testing purposes. The inputs used are the temperatures of 19 trays and target outputs are the compositions of the four components in the distillate. The Adaline and LM soft sensors are designed and trained to estimate the distillate composition of reactive distillation process. The trained sensors are then tested by using test inputs different from those used in training. The estimated distillate composition by the two sensors for reactive process is shown in Fig. 2(a)-(d). It is observed from estimated results that the estimation made by Adaline is almost coinciding with the simulated results. The estimated results using LM technique are slightly deviating from the original simulated results. The deviation of estimated results is due to the reason that LM technique suits more for the highly complex and nonlinear relations. In this case the complexity is slightly reduced because the number of outputs is less. It is also observed that the Adaline estimator takes extremely less time as compared to the LM estimator. The performance parameters for both the estimators are shown in Table 1.



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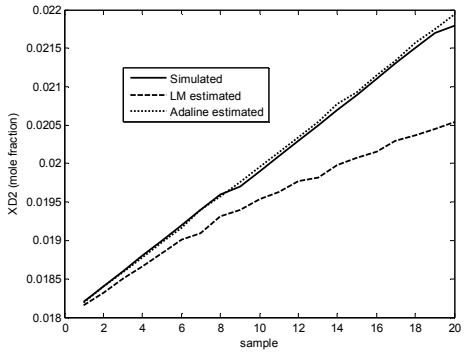

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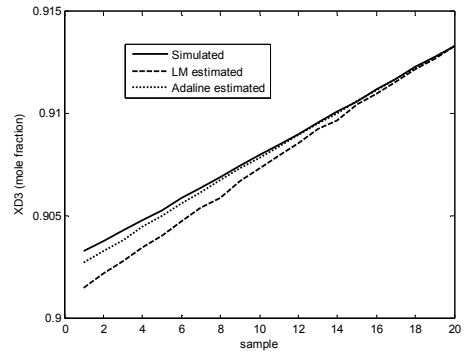

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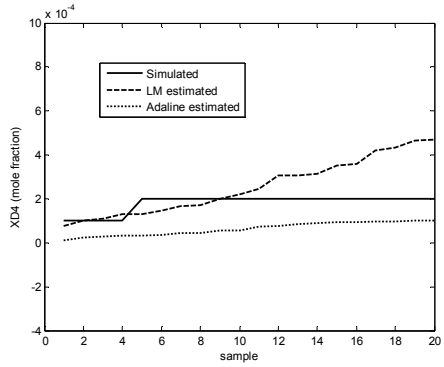
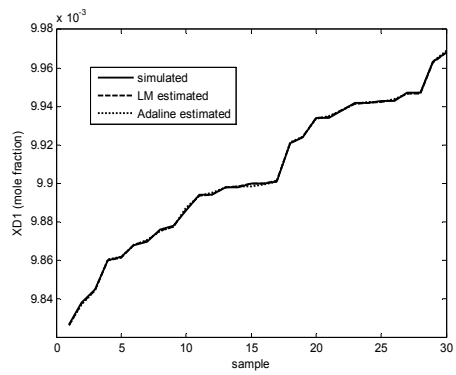


(d)

Fig. 2 Estimated composition of distillate product (a) XD1 (b) XD2 (c) XD3 (d) XD4

3.2 Multicomponent Distillation Process

The multicomponent distillation column under consideration is having 15 trays, a reboiler to vaporise the mixture and a condenser to cool the overhead vapour. Tray 5 is used as feed tray. In distillation, a liquid mixture is fed on the feed tray and the mixture is stored in reboiler. The heat is introduced in the reboiler to produce vapour. The vapour starts flowing from the reboiler to top tray and then to condenser through stripping and rectifying section. During initial start-up period, the column operates under total reflux condition in which vapour from the top of the column is condensed and returned to the column through reflux drum. During the column operation under total reflux condition, the concentration of the lightest component builds-up on the upper trays of the column and the concentrations of the intermediate component and heaviest component decreases in the top of the column but increases in the still pot. When the concentration of the lightest component in the distillate reaches its specified purity level, then the distillate product withdrawal begins.



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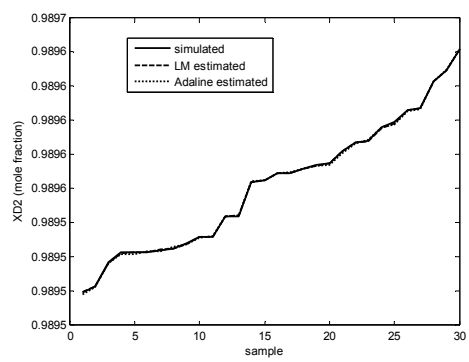

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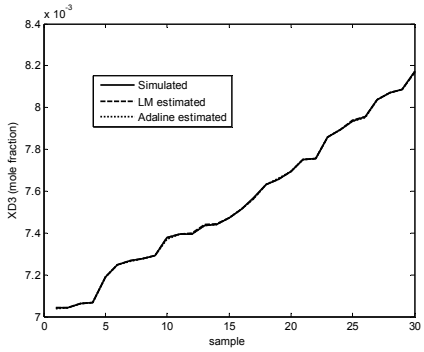

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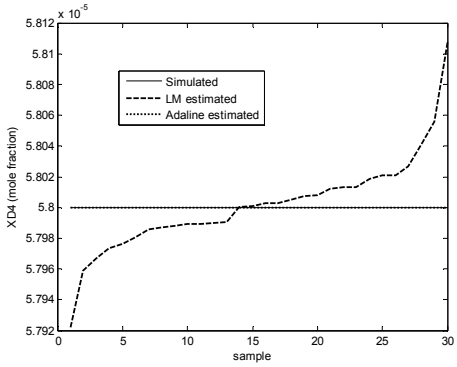

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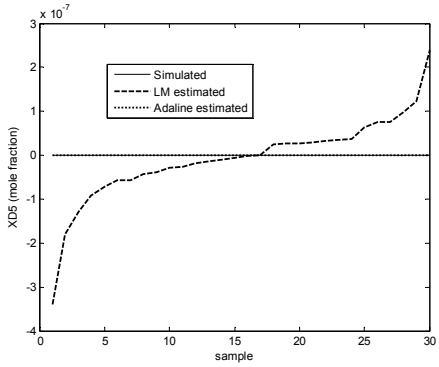
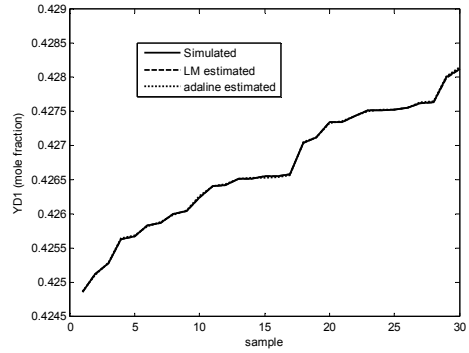


(e)

Fig. 3 Estimated Composition of Liquid composition in Distillate (a) XD1,(b) XD2, (c) XD3 (d) XD4, (e) XD5

The quality of distillate must be maintained within the specified limits which require the composition measurement. The measurements made by the composition analysers are difficult due to time delay and maintenance reasons. Therefore the product composition is measured with the help of soft sensors. In the present work two soft sensors are designed for estimation of product composition. The data used for training the soft sensors is acquired by simulating the mathematical model of multicomponent distillation process for variable heat input. In this case temperature profile (temperature of 15 trays, reboiler and condenser), heat input, reboiler pressure and reflux flow rate are used as inputs and liquid and vapour compositions of five components in distillate are the target outputs for the soft sensors. The data set so generated is used for training and testing of the designed soft sensors. The test results obtained are shown in Fig.3 and Fig.4.



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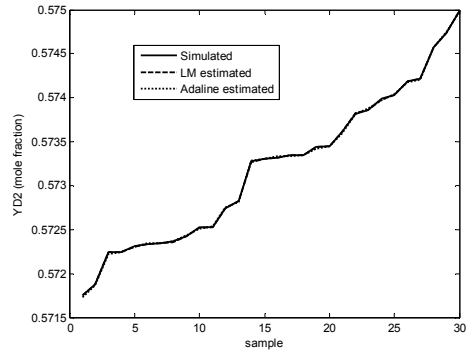

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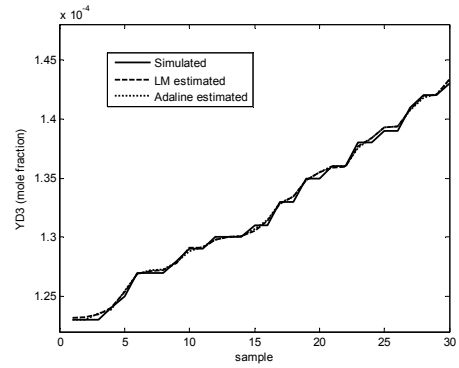

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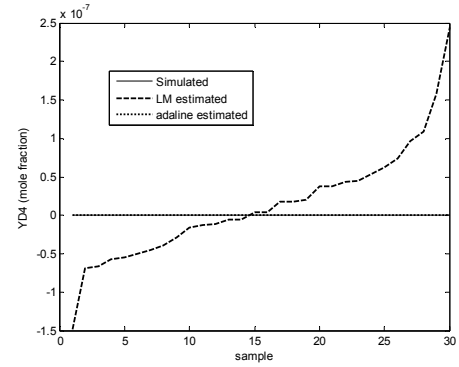

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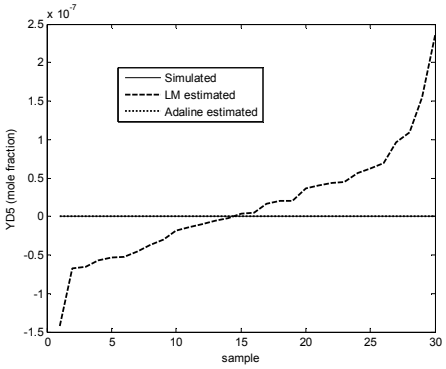

(e)

Fig. 4 Estimated vapour composition in Distillate (a) YD1,(b) YD2, (c) YD3 (d) YD4, (e) YD5

It is observed from the estimated results that the Adaline soft sensor estimates the product composition quite accurately as compared to the LM soft sensor. In the case where the composition is very less the LM soft sensor is not able to predict the composition correctly, whereas Adaline soft sensor provides a very good estimation. It is also observed that Adaline being a single layer takes negligibly less time for training than the LM network. The memory space used, is also very less in case of Adaline network as the number of elements in the network is less. The comparison of performance parameters of the two soft sensors is shown in Table 1.

Table 1. Performance indices of estimators

Process	Estim-ator	Architecture	MSE(test)	Execution time (sec)
Multi-component Distillation	Adaline	20-10	2.9092e-11	0.078
	LM	20-15-15-10	1.4212e-12	88.79
Reactive Distillation	Adaline	19-4	1.9409e-8	0.016
	LM	19-12-12-4	3.9629e-07	9.117

4. CONCLUSION

In the present work, an adaptive linear network is used to design a soft sensor for estimating the product composition from temperature profile of the process. The Adaline network is similar to the perceptron but the transfer function is linear rather than hard limiting. The proposed estimator is a single layer Adaline and it uses the supervised learning algorithm known as least mean square algorithm or delta learning rule. A LM based ANN estimator is also designed for comparative study. It is observed from the results that in case of reactive distillation process the Adaline soft sensor gives more accurate results as compared to the LM soft sensor. In case of multicomponent distillation process the performance of the LM soft sensor is not up to the mark for the case where composition is very less, whereas the estimated results obtained by Adaline soft sensor coincide with the simulated composition. The Adaline soft sensor being a single layer network requires extremely less time and memory space during training. Therefore, it is concluded from the observations that the Adaline soft sensor proves to be more efficient than LM estimator in terms of accuracy, training time and memory space required for training.

Nomenclature:

η=Learning parameter for neural network

μ_k= Eigenvalue of approximate Hessian matrix

a_q= Desired qth output of the function

$e_{k,q}$ = qth Error between target and input of kth element

$\boldsymbol{H}$ =Hessian Matrix

$\boldsymbol{J}(x)$ = Jacobian matrix

n_i^m =Sum of multiplication of input and weight of ith layer

$\tilde{s}_{i,h}^m$ =Marquardt sensitivity for a general layer

$\tilde{s}_{i,h}^M$ =Marquardt sensitivity at final layer

$\tilde{s}^M$ =Total Marquardt sensitivity matrix

t_q = qth target value of the function

Δx_k =Change in the old guess values of x_k

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