

## Neuro-fuzzy Inference System for Modeling Equilibrium Ratio for Heptanes-plus Fraction

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**ABSTRACT:** Equilibrium constant has many applications in solving problems in reservoir engineering and petroleum processing. Various correlations are available for estimating K- values for heptanes plus fractions. These correlations can be classified into simple and complicated. However these correlations are not able to predict K values adequately for a wide range of conditions. They lose validity in specific range of pressure and temperature and exhibit some error. In this work neuro-fuzzy modeling techniques (ANFIS) is developed to predict K- values for heavy fractions. A large collection of K- values data points (more than 1340 data points) were extracted from experimental 570 PVT reports using the principal of material balance are used in developing the neuro- fuzzy model. 80% of the data points were used to train ANFIS model and 20% of data sets were used to validate, and test the model. Statistical analysis (average absolute percent error, correlation coefficient, standard deviation, maximum error, minimum error, etc.) is used for comparison the proposed model with empirical correlations. Graphical tools have also been utilized for the sake of comparison the performance of the new model and experimental data. Results showed that the new hybrid neural fuzzy model outperforms some available empirical correlations.

**KEYWORDS:** Heptanes plus, Neuro-fuzzy model, K- values, Empirical correlations, Equilibrium ratio.

### 1 INTRODUCTION

Equilibrium constant is an important factor in many petroleum engineering calculations such as simulation of enhanced oil recovery, design of surface oil and gas production operations. The basic phase equilibrium calculations include the dew point pressure, bubble point pressure and separator calculations.

Because the plus fraction is a complex mixture of different components, the equilibrium ratio for plus fraction often have different behavior from individual components of the hydrocarbon system. Several methods have been proposed for calculating equilibrium constant. These correlations ranged from simple to complicated with multiple dependent variables. Some methods use graphical procedure (Campbell's [6] and Hoffmann's [20] methods). Katz [17] suggests method for determining K-values for heptanes plus fraction by taking 15 % of K-value of heptanes. These correlations widely used because they are adapted to calculations, less costal time and time consuming. However they can't be used for wide range of pressure, temperature and fluid system parameters in addition to their inaccuracy. For calculating K-value these correlations was improved [11] by tuning them for practical reservoir fluid because of different composition of oil from region to region. But it still exhibits some error. This variation in the K-value of hydrocarbon fraction can cause error in phase equilibrium problems in reservoir and process engineering.

Due to advance in computer calculation of k- value is performed by equation of state (EOS) using powerful computer and modern software. For using EOS model it is necessary to use different correlation for calculating EOS parameters such as  $P_c$ ,

$T_c$ ,  $\omega$ , etc.). EOS characterized by its simplicity, consistency, and accuracy when properly tuned. However EOS requires tuning the parameters against experimental data. Calculations with equation of state are limited by the large number of functions. Furthermore, calculating using EOS require extensive amount of computational time, may have the convergence problem, time consuming and complex where large number of K-values are required.

Several correlations may be used to estimate the critical properties of heptanes plus fractions. Selecting proper values for these parameters is very important because slightly difference in these parameters can cause significant difference in results. A genetic algorithm can be used as effective tool to determine the optimum critical properties of heptanes plus [19]. An increase in deviation of k-values of heptanes plus fraction from experimental data may be due to method of characterization.

In this study neural fuzzy model for predicting equilibrium ratio for heptanes plus fraction was developed.

## 2 WATSON CHARACTERIZATION FACTOR

The physical properties of the plus fractions in hydrocarbon mixtures are essential in performing phase equilibrium calculations. Characterization the plus fractions in terms of their critical properties and acentric factors can be provided by using one of the proper methods [16].

Three approaches commonly are used to generate properties of the plus fractions: generalized correlations, correlations based on the PNA determination, and graphical correlations. These three techniques of characterizing the heavy petroleum fractions are discussed in [18].

In many cases for the heavy fraction there are no boiling point or molecular weight distributions, and only specific gravity and molecular weight may be available. The characterization factor was introduced by Watson [13] to describe qualitatively the relative parafinicity of petroleum products. Physical properties, such as molecular weight and specific gravity, may be measured for the heavy fraction. Watson characterization factor can be used to describe heptanes plus fraction according to the equation [13]:

$$K_w = \frac{T_b^{1/3}}{\gamma}$$

This characterization factor was introduced to relate the molecular weight, specific gravity and boiling point temperature which considered the key properties of petroleum fractions. Thus Watson characterization factor can be an important parameter in the correlation of equilibrium constant.

In present work we use approach that Watson factor may be introduced as a correlating parameter which used as input for estimating K-values of heptanes plus fraction.

## 3 MATERIAL BALANCE

Material balance was performed for laboratory test (constant volume depletion(CVD), differential liberation (DL) and separation test for one, two, three, and four stage flash separation (sour and sweet gas). These calculations allow us to determine liquid composition at separator conditions and hence estimate the equilibrium K-values experimentally [14].

## 4 DATA ACQUISITION

More than 1340 Data points from 570 PVT reports collected from different regions in Middle East and published data in literature were used for developing the model.

Statistical descriptions of these data are given in the table below.

Table 1. Statistical summary of data used for model development.

Parameter	Maximum	Minimum	Average	ST-deviation
Separation pressure, psia	765	15	94.61	107.38
Separation temperature, °F	195	70	108.6	21.22
Specific gravity	1.032	0.795	0.888	0.03
Molecular weight of heptanes plus	534	162	274	49.31
K-factor	0.066	1.310 <sup>-7</sup>	0.007	0.00793
Kw	12.75	11.03	11.8	0.12689
Heptanes plus, mole percent	86.10	18.50	46.62	13.80

## 5 NEURO FUZZY MODEL ARCHITECTURE

Fuzzy inference [7] is a process of mapping from a given input to an output using the fuzzy set methods. The basic idea behind neuro- fuzzy combination is to design a system that use a fuzzy system represents knowledge in an interpretable manner and have the learning ability derived from a neural network to adjust its membership functions and parameters in order to enhance the system performance. Neuro-fuzzy methods offer good capabilities to deal with high noisy data. Neuro-fuzzy approach combines the advantages of both neural network and fuzzy logic, have been emerged as a successful practical technology application including prediction of oil properties.

Neuro-fuzzy model can achieve a higher accuracy within a relatively shorter training time comparing with neural network system. The main disadvantages of both individual systems could be avoided, i.e., the black box behavior of neural networks and the problem of selecting suitable membership values for FISs. Architecture of ANFIS is determined by preliminary testing. ANFIS produced 42 fuzzy rules. The model was evaluated using the testing data by utilizing the approach, Takagi-Sugeno-Kang (TSK)[9]. ANFIS required 50 training epoch to reach a Root-mean squared error (RMSE) of 3.98 10<sup>-6</sup>. The stopping criterion is either completion of the given training epoch or reaching 0.00001 mean classification error for the training data set. Before training data pre-processing was performed to transform data into suitable form to the ANFIS input. All data were normalized, i.e. all values of attributes in the dataset has been changed to contain values in the interval (0,1).

The approach used in this study is Maximum- Minimum normalization techniques. This technique performs a linear transformation on the original data.

Subtractive clustering was performed on a dataset. The number of clusters determines the number of rules and membership functions in the generated ANFIS.

To generate a model from data cluster radius was specified. The cluster radius indicates the range of influence of a cluster when the data space as a unit hypercube is considered. The ANFIS could be optimized by adjusting cluster radius so as to reduce error between the actual and predicted outputs. This allows the fuzzy system to learn from the data for modeling so optimal structure of neuro- fuzzy model is obtained.

The input to INFIS is separation pressure, separation temperature, molecular weight of heptanes plus, specific gravity of heptanes plus and Watson characterization factor. Model has only one output K-values.

A total of 1344 data sets are used for building the model. Dataset partitioning was done by dividing the data into two different sets, training sets (80%), validation sets (20%). Statistical parameters for training and validation data sets are given in Tables (2) and (3).

Table 2. Statistical descriptions of the input data used for training

Parameter	Maximum	Minimum	Average	ST-deviation
Separation pressure, psia	759.31	14.90	92.03	107.04
Separation temperature, °F	183.63	69.49	105.44	17.59
Specific gravity	1.04	0.80	0.89	0.03
Molecular weight of heptanes plus	530.03	163.78	273.45	50.04
K-factor	0.08	0.01	0.02	0.01
Kw	12.67	10.96	11.72	0.13

Table 3. Statistical description of the input data used for validation

Parameter	Maximum	Minimum	Average	ST-deviation
Separation pressure, psia	511.17	14.90	101.72	105.01
Separation temperature, °F	193.56	74.45	116.62	29.19
Specific gravity	1.02	0.80	0.89	0.03
Molecular weight of heptanes plus	463.53	160.80	266.10	44.22
K-factor	0.06	0.01	0.02	0.01
Kw	11.92	11.36	11.71	0.08

## 6 RESULTS AND DISCUSSION

The best available empirical correlations were tested in this work to obtain prediction of the K-values for all data. Comparison of statistical analysis of the different used correlations for estimating equilibrium ratio against extracted K-values for the heptanes-plus is shown in Table 4.

Table 4. Performance of empirical correlations using all data

Correlation	Wiston-Torp	Standing	Wilson
ARE	99.84	-70.6	99.90
AARE	99.84	98.2	99.90
Minimum error	91.94	0.0	91.64
Maximum error	100	694.2	100
ST-deviation	0.544814	104.519	0.39
R	0.339	0.565	0.381

From Table 4 it can be observed that Standing correlation have best performance among all three correlations used for predicting K-values.

Calculation of K-values by standing was performed using Standing characterization factor [1] for heptanes plus fraction. For calculation by Wilson and Whiston-Torp correlation characterization of heptanes-plus was performed by Riazi and Daubert correlation [5] to calculate  $T_b$ ,  $T_c$ , and  $P_c$ .

Wilson [2] and Whiston [3] models approximately have the same range of statistical error. The similarity in accuracy may be attributed to using a general correlation (Riazi and Daubert) to calculate  $T_b$ ,  $T_c$ , and  $P_c$ .

Prediction of K-values by standing model also was performed using Riazi and Daubert instead of using the correlation indicated by Standing which characterize the plus fraction as a function of average carbon number, n. This resulted in absolute relative percent error equal to 99.7 %.

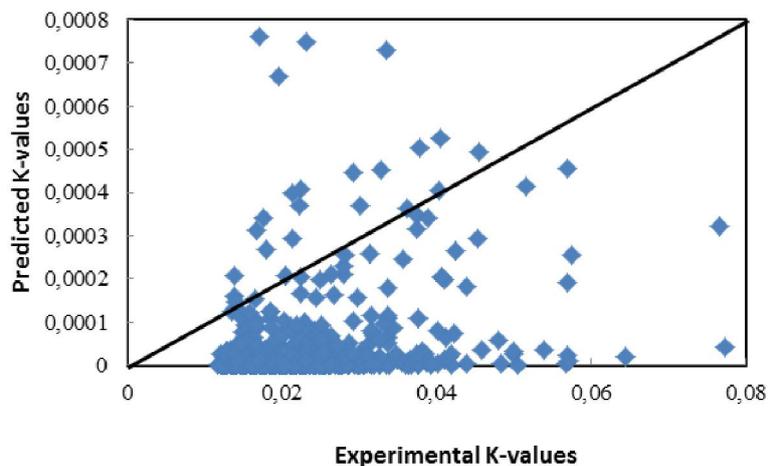


Fig. 1. Crossplot of experimental and predicted K-values (Wilson correlation)

The cross plots of estimated against the actual values using the three empirical correlations are shown in Figures (1)-(2). They indicate poor of performance in terms of correlation coefficient.

In general, Wiston-Torp and Wilson correlations underpredict experimental K-values. Standing’s correlation [1] tends to overpredict experimental K-values at pressures below 65 psia.

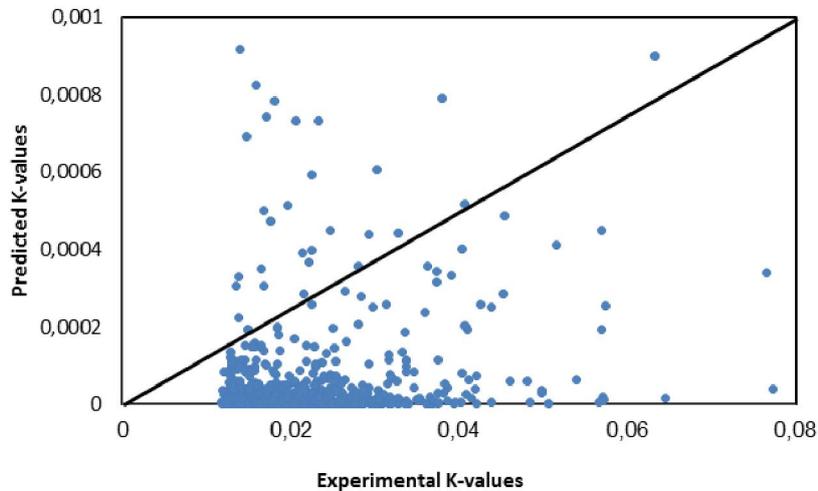


Fig. 2. Crossplot of experimental and Predicted K-values (Whiston-Torp)

Table 5 lists statistical comparison of predicted K-values by using the proposed neuro-fuzzy model with the experimental values. It is indicated that developed model gives best results compared with empirical correlations.

Fig. 3 shows scatter plot of calculated compared to laboratory measurement of K-factors. It is indicated the accuracy of the results presented in this figure far exceeds those of any correlations. Predicted and fact data of K-values for training and validation process respectively are presented in Figures (4) and (5). Figures (7) and (8) give behavior of the average percent error for training and testing data. Crossplots of predicted and experimental data for validation and training are shown in Figures (6) and (9), respectively.

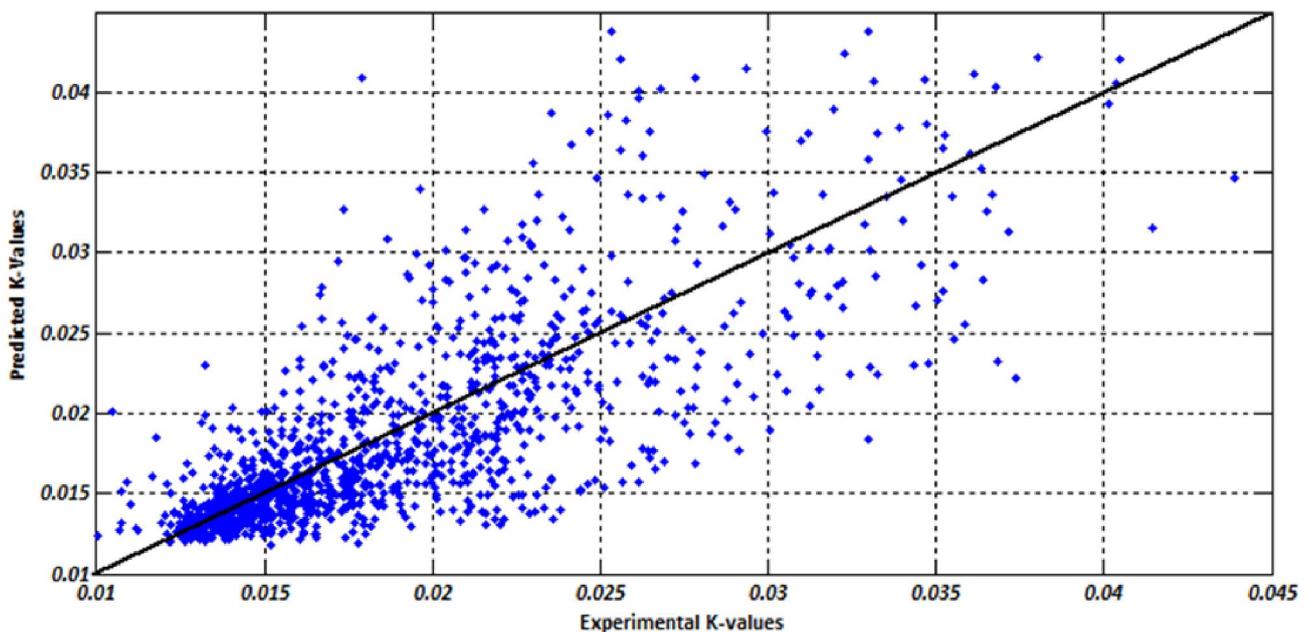


Fig. 3. Crossplot of experimental and predicted K-values of all data (This study)

Table 5. Statistical parameters for proposed neural fuzzy model

Parameter	Training	validation	All
Minimum error	0.00	0.16	0.02
Maximum error	79.49	69.50	79.13
ARE	-3.74	-1.68	-3.76
AARE	14.10	15.99	14.78
ST-deviation	14.46	13.61	14.33

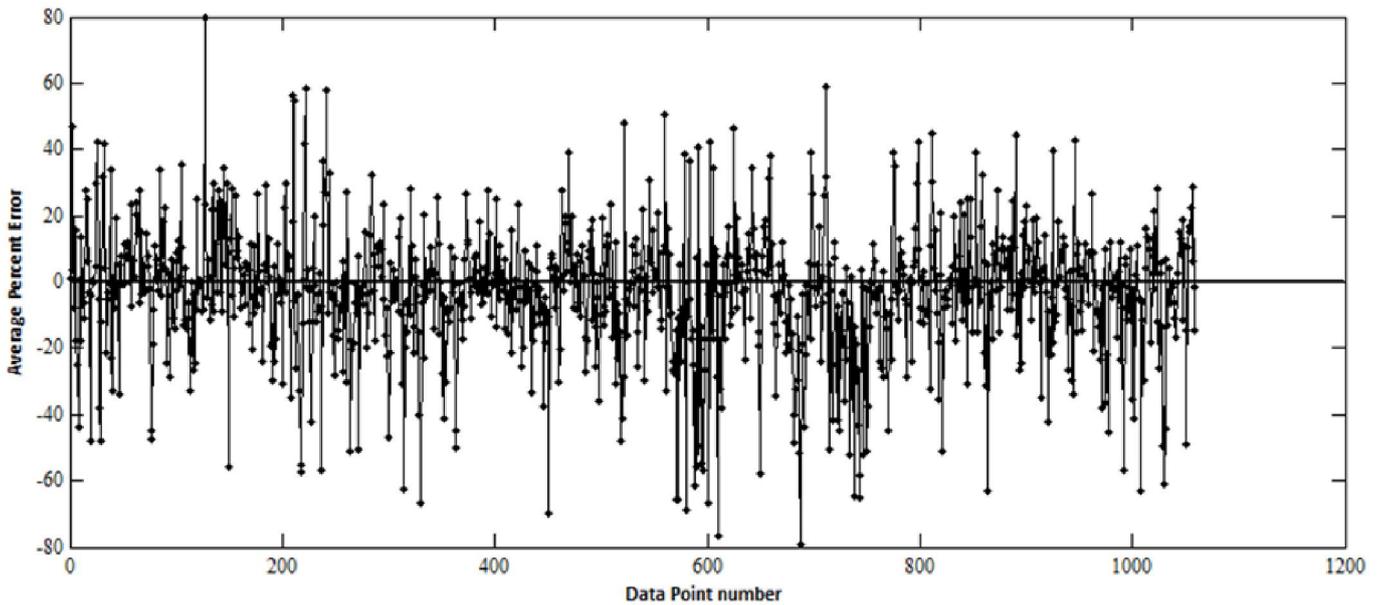


Fig. 4. Error graph for Training Set (Neuro-fuzzy model)

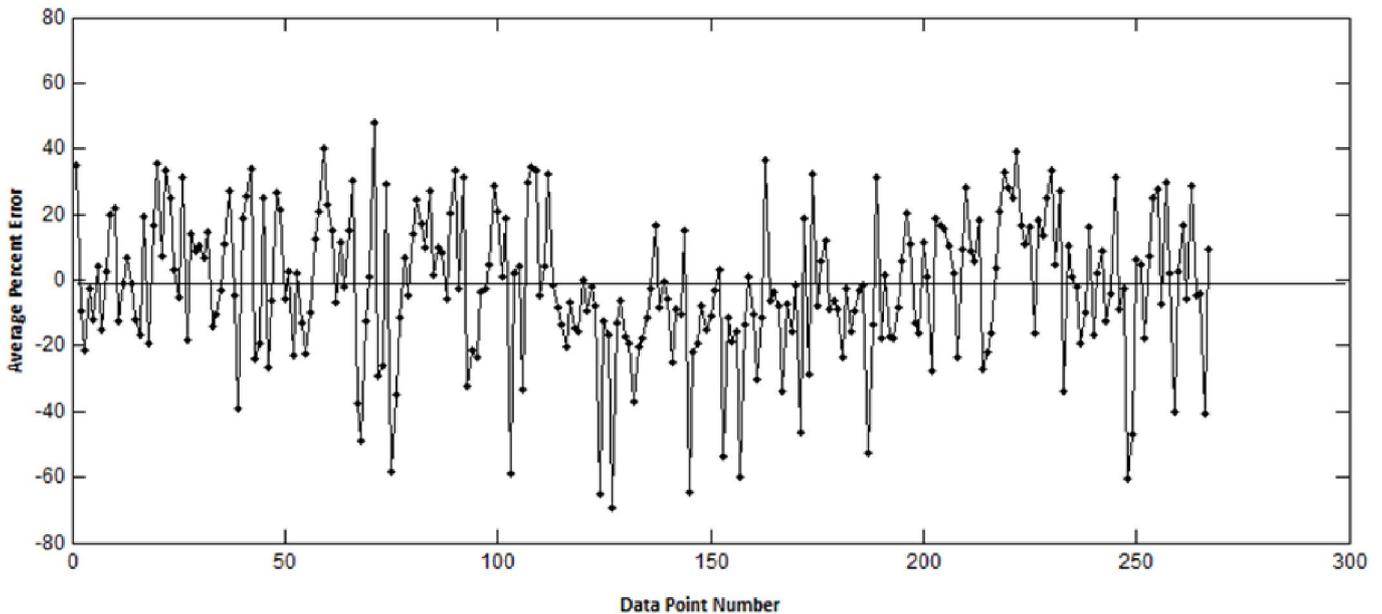


Fig. 5. Error graph for Validation Set (Neuro-fuzzy model)

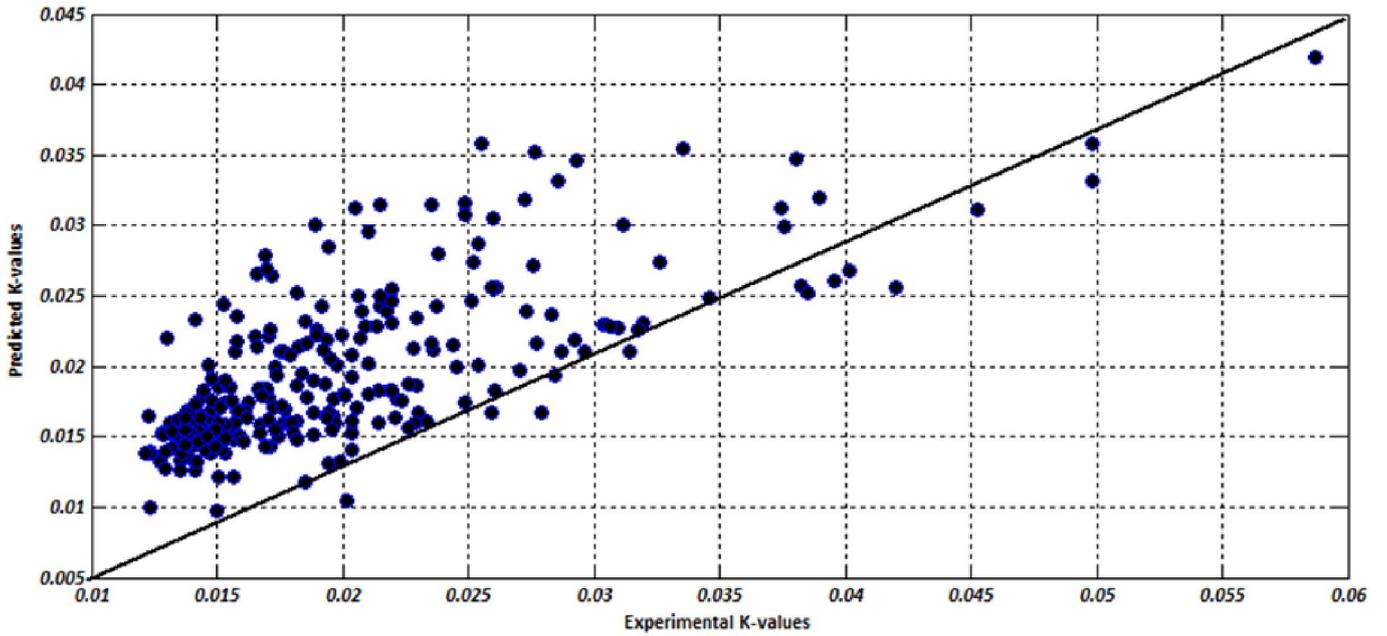


Fig. 6. Crossplot of experimental and predicted K-values for validation

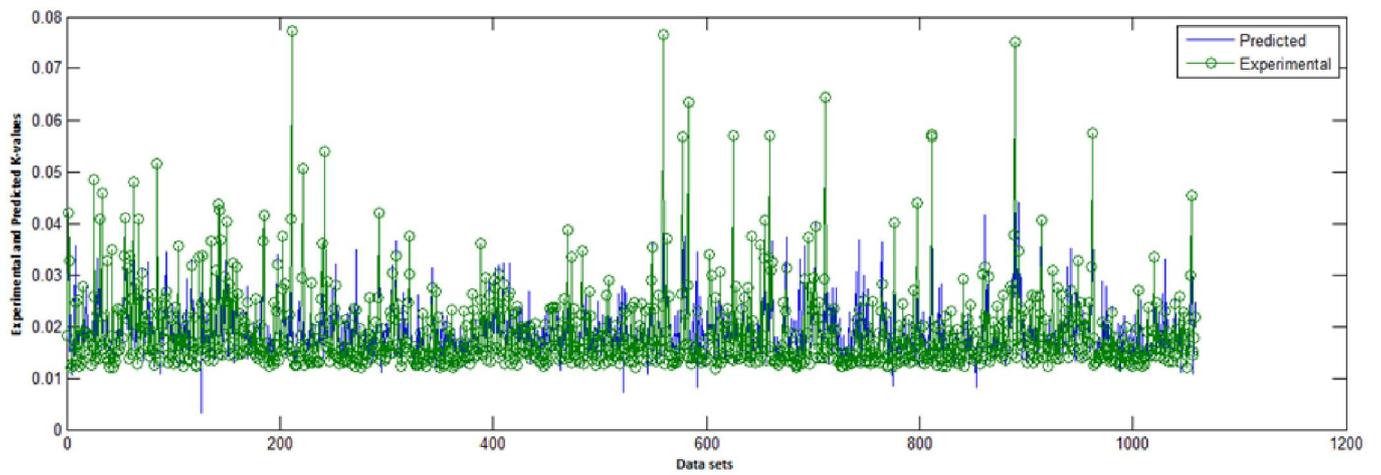


Fig. 7. Comparing Experimental and predicted k-values for Training (This study)

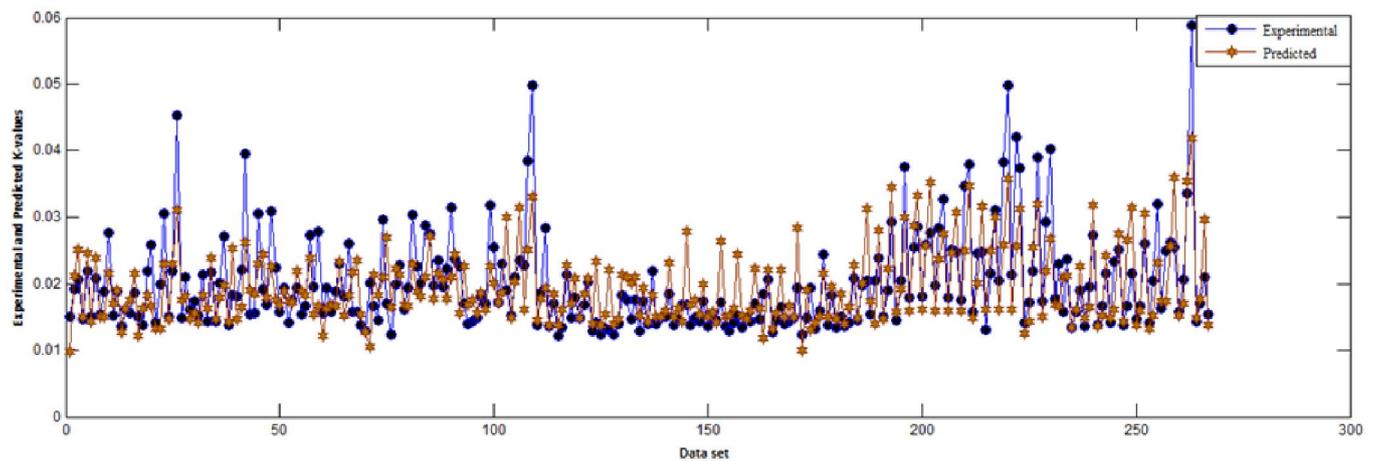


Fig. 8. Comparing Experimental and predicted k-values for validation (This study)

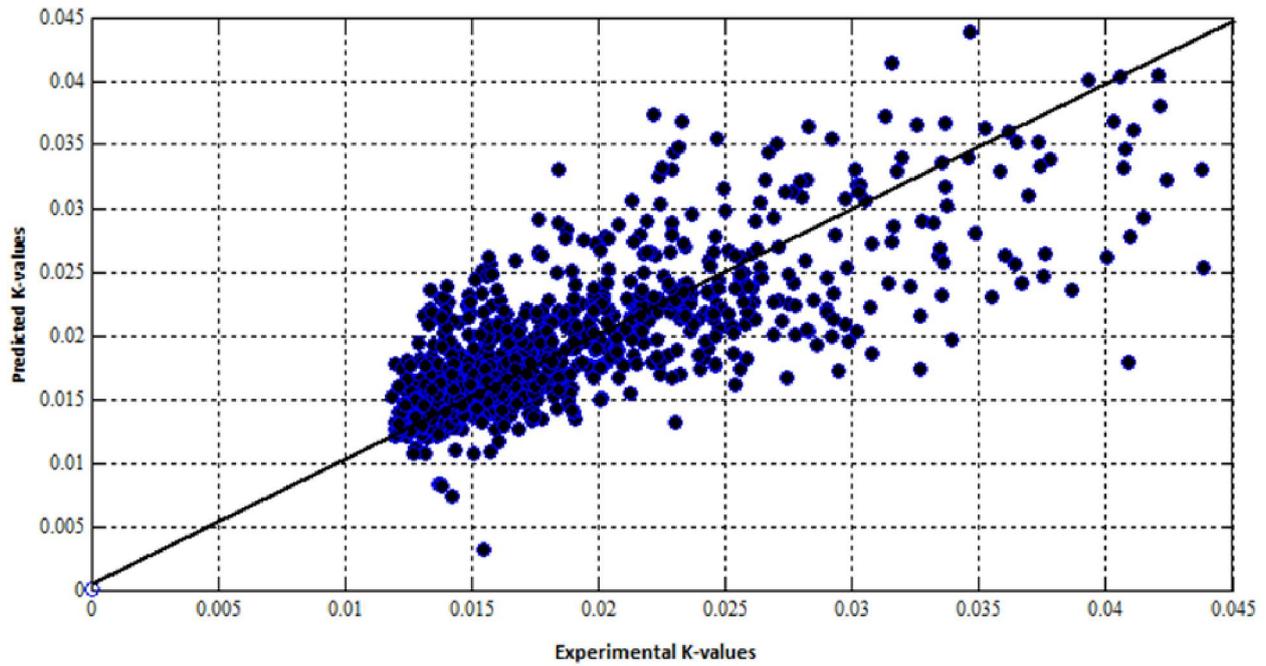


Fig. 9. Crossplot of experimental and predicted K-values for training

The Rule Viewer displays a roadmap of the whole fuzzy inference process (Fig.10).

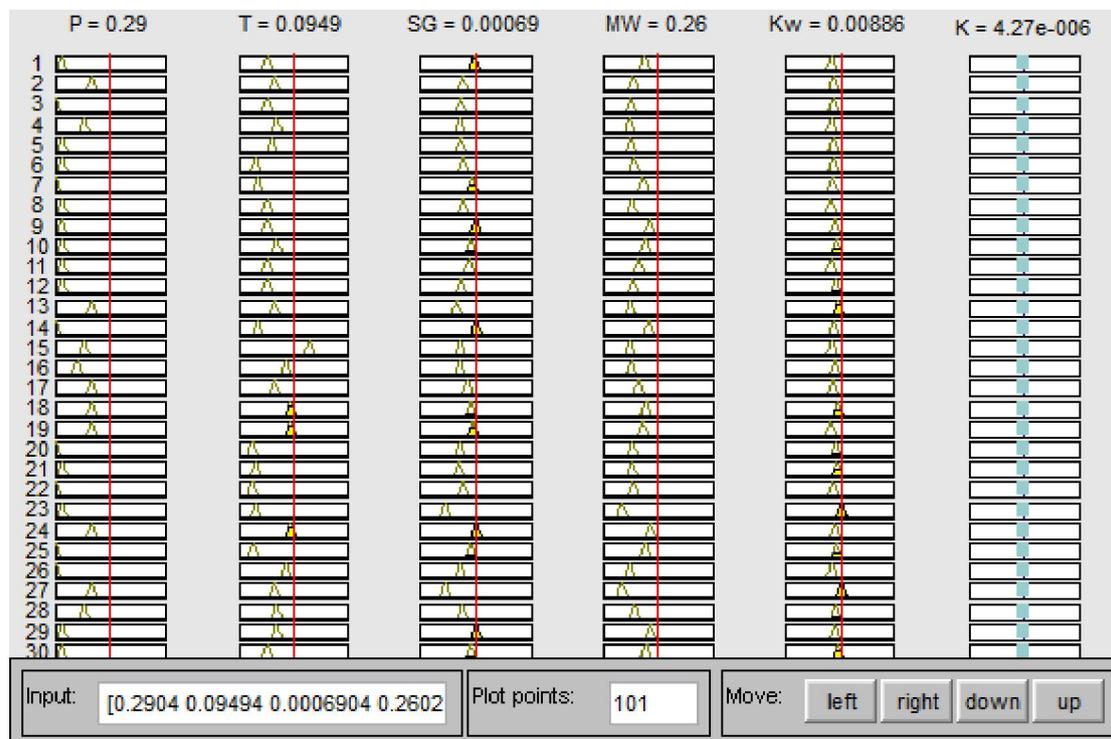


Fig. 10. Rule viewer of Neuro-fuzzy model

## 7 CONCLUSION

- A new hybrid neural fuzzy model was developed to predict equilibrium constant of heptanes plus fraction. Validation of the method was done by comparison the model with empirical correlation which indicate that the proposed model outperform others empirical correlations.
- The developed model can be used only within the range of used data.

## NOMENCLATURE

$p_c$  = critical pressure, psia

$T_c$  = critical temperature, °R

$\omega$  = acentric factor

$T_b$  = normal boiling point, °R

R = correlation coefficient

Kw = Watson characterization factor

PNA = (Paraffins- naphthenes- aromatics)

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