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Investigation of Artificial Neural Networks Performance to Predict Net Heating Value of Crude Oil by its Properties

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***Abstract*—**The aim of this research is to use artificial neural networks computing technology for estimating the net heating value (NHV) of crude oil by its Properties. The approach is based on training the neural network simulator uses back-propagation as the learning algorithm for a predefined range of analytically generated well test response. The network with 8 neurons in one hidden layer was selected and prediction of this network has been good agreement with experimental data.

***Keywords*—**Neural Network, Net Heating Value, Crude Oil, Experimental, Modeling.

I. Introduction

NET heat of combustion $[Q_n(Mj/kg)]$ is defined the quantity of energy released when a unit mass of fuel is burned at constant pressure, with all of the products, including water, being gaseous. The fuel can be either liquid or solid, and contain only the elements carbon, hydrogen, oxygen, nitrogen, and sulfur. The products of combustion, in oxygen, are carbon dioxide, nitrogen oxides, sulfur dioxide, and water all in the gaseous state.

Gross heat of combustion, $[Q_g(Mj/kg)]$ is defined the quantity of energy released when a unit mass of fuel is burned in a constant volume enclosure, with the products being gaseous, other than water that is condensed to the liquid state. The fuel can be either liquid or solid and contain only the elements carbon, hydrogen, in oxygen, are gaseous carbon dioxide, nitrogen oxides, sulfur dioxide, and liquid water.

In SI the unit of heat of combustion has the dimension J/kg, but for practical use a multiple is more convenient. The MJ/kg is customarily used for the representation of heats of combustion of petroleum fuels. The net heat of combustion is represented by the symbol Q_n and is related to the gross heat of combustion (Q_g) by the following equation [1]:

$$Q_n(\text{net}, 25^\circ C) = Q_g(\text{gross}, 25^\circ C) - 0.2122 \times H \quad (1)$$

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$Q_n(\text{net}, 25^\circ C)$: Net heat of combustion at constant pressure, MJ/kg

$Q_g(\text{gross}, 25^\circ C)$: Gross heat of combustion at constant volume, MG/kg

H: Mass % of hydrogen in the sample

II. Net Heating Value Measurement

A. Significance and Use

The heat of combustion is a measure of the energy available from a fuel. The knowledge of this value is essential when considering the thermal efficiency of equipment for producing either power or heat.

The heat of combustion is designated as one of the chemical and physical requirements of both commercial and military turbine fuels and aviation gasoline's.

The mass heat of combustion, the heat of combustion per unit mass of fuel, is a critical property of fuels intended for use in weight-limited craft such as airplanes, surface effect vehicles, and hydrofoils. The range of such craft between refueling is a direct function of the heat of combustion and density of the fuel.

The net heat of combustion is a factor in the performance of all aviation fuels. Because the exhaust of aircraft engines contains uncondensed water vapors, the energy released by fuel in vaporizing water cannot be recovered and must be subtracted from gross heat of combustion determinations to calculate net heat of combustion. For high performance weight-limited aircraft, the net heat of combustion per unit mass and the mass of fuel loaded determine the total safe range. The proper operation of the aircraft engine also requires a certain minimum net energy of combustion per unit volume of fuel delivered.

B. Empirical Method

There is a method that is purely empirical, and it is applicable only to liquid hydrocarbon fuels derived by normal refining processes from conventional crude oil which conform to the requirements of specifications for aviation gasoline or aircraft turbine and jet engine fuels of limited boiling ranges.

The empirical method is intended for use as guide in cases where an experimental determination of heat of combustion is not available and cannot be made conveniently, and where an estimate is considered satisfactory. It is not intended as a suitable for experimental measurement of heat of combustion.

Because the heat of combustion of hydrocarbon fuel-mixtures are slowly varying function of the physical properties of the mixtures, the heat of combustion of the mixtures can often be estimated with adequate accuracy from simple field tests of density and aniline point temperature, without the elaborate apparatus needed for calorimeter method.

The empirical quadratic equation for the net heat of combustion of a sulfur- free fuel was derived by the method of lest squares from accurate measurements on fuels, most of which conformed to wide range and were chosen to cover a range of values of properties. Those fuels not meeting specifications were chosen to extend the range of densities and aniline-point temperatures above and below the specification limits to avoid end effects. The sulfur correction was found by a simultaneous least squares regression analysis of sulfur-containing fuels among those tested.

C. Procedure

1- Determine the aniline point temperature of the sample to the nearest 0.05 °C as described in Test Methods D 611 [3]
2- Determine the density at 15 °C of the sample to the nearest 0.5 kg/m3 as described in Test Method D 941, Test Method D 1298, or Test Method D 4052 [4].
3- Determine the sulfur content of the sample to the nearest 0.02 mass % sulfur as described in Test Method D 129, Test Method D 1266, Test Method D 2622, or Test Method D 3120 [5]

D. Calculation

Insert the measured values in equation 2 and calculate Qn, the heat of combustion at constant pressure on a sulfur-free basis.

$$Q_n = 22.9596 - 0.0126587\,A + 26604.9\left(\frac{1}{\rho}\right) + 32.622\left(\frac{A}{\rho}\right) - 6.69030\times10^{-5}\,(A)^2 - 9217760\left(\frac{1}{\rho}\right)^2 \quad (2)$$

ρ : Density at 15 °C, kg/m^3

A : Aniline point temperature, °C

Q_n : net heat of combustion on sulfur free basis, MJ/kg

III. Neural Networks Modeling

A feed-forward back-propagation artificial neural network is chosen in the present study since it is the most prevalent and generalized neural network currently in use and straightforward to implement. The architecture of the neural network used in this paper is shown in Fig. 1. It has three input layer, one output layer, and one hidden layer. The neurons in hidden layer are represented by a weight matrix W, a bias vector B, a net input vector E, and an output vector O. The weights determine the strength of the connections between interconnected neurons. Every node in any hidden layer sums its weighted inputs, adds the bias constant, and then the output value of this node is calculated by applying a chosen function (known as a basis, activation, or transform function) to the weighted sum. In this manner, input values are passed through the network topology and transformed into one or more output values. The output values are then compared to the desired values to adjust the weights and bias in the nodes. Thus, the final output from the node is calculated using equation 1.

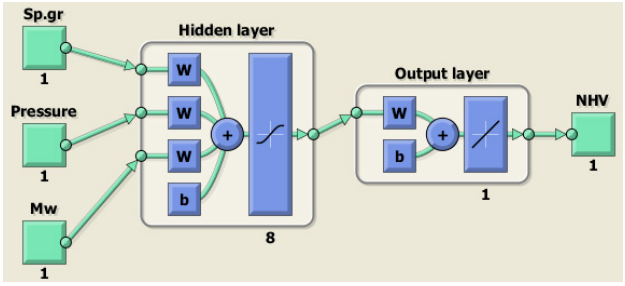

Fig. 1 Architecture of a multiple-layered neural network with a single hidden layer

$$y = f\left[w_0 + \sum_{j=1}^{n_2} w_j f_j \left(\upsilon_{0j} + \sum_{i=1}^{n_1} \upsilon_{ij} x_i \right) \right] \quad (3)$$

where y is the output variable, x is input variable, w and t are the connection weights, n1 is the dimension of the input vector, and n2 is the number of hidden neurons. In this study, a sigmoid function is used as the transformation function:

$$f(x) = \frac{1}{1 + \exp(x)} \quad (4)$$

The backward propagation step calculates the error vector, E by comparing the calculated outputs, y and the target values, d by equation 5:

$$E = y - d \quad (5)$$

The gradient descent method is used to minimize the total error on patterns in the training set. In gradient descent, connection weights are changed in proportion to the negative of an error derivative with respect to each weight:

$$\Delta w_j = -\alpha \frac{\partial E}{\partial w_j} = \alpha \left[-\frac{\partial E}{\partial y} f'(NET) \right] x_j = \alpha\, \delta_y\, x_j \quad (6)$$

where α is a learning rate, and ∂ is an error signal. New sets of connection weights are iteratively calculated based on the error values until a minimum overall error is obtained. The connection weights are analyzed after training. These weights relate to the average contributions of each input log to the network by following equation [6]:

$$C_i = \frac{\sum_{j=1}^{n_2} w_{ij}}{\sum_{k=1}^{n_1}\sum_{j=1}^{n_2} w_{kj}} \quad (7)$$

where C_i is the average contribution of input variable i and w_{ij} is the connection weight from input neuron i to hidden neuron j. This intelligent computing technique can help engineers in solving problems that have not been solved by traditional and conventional computing methods. Neural networks do not require the specification of a structural relationship between the inputs and outputs unlike statistical regression analysis.

One of the most common problems in training an ANN is over fitting; where the error on the training set is reduced but the error for predictions using new data is large. This problem usually occurs with large networks that have few training examples. However, by dividing the data into two sets (training and testing) and selecting the best structure among them, over fitting can be avoided [6]. In the present study, 80% of the total data was used for training and testing: 60% for training and 20% for testing. The remaining 20% of the total data represented the verification or production set. The verification set is used to evaluate the accuracy of the newly built network by providing the network with a set of data that it has never seen. Prior to any modeling, all data were scaled to the range [0–1]. Once the training process converged, the testing data set was presented to the network. If the testing presented good agreement between the actual and the estimated net heating value of crude oil (NHV), the bias and weight matrices were saved and kept aside. If not, the realization was canceled. This process was repeated several times until a satisfactory number of realizations with good testing results were achieved. In this work, the network is trained for maximum 200 epochs.

IV. Experimental Data

Net heating value of 88 different well in three zones was measured and is shown in Table I.

TABLE I
EXPERIMENTAL DATA OF WATER CONTENT IN CRUDE OIL

number	Pressure (bar)	Specific Gravity	M_W	NHV (Exp)	NHV (Estimated)	Error (%)
1	44	0.6719	388	1058.4	1052.199054	0.585879217
2	47	0.6625	382	1039.9	1043.134368	-0.311026809
3	48	0.6651	384	1048.1	1059.990131	-1.134446205
4	45.7	0.6442	372	1019.5	1018.77464	0.071148613
5	35.5	0.6703	388	1052	1051.317578	0.064868971
6	45	0.6597	382	1041.9	1038.660361	0.310935684
7	48	0.661	382	1043.3	1045.498645	-0.210739525
8	45	0.6661	384	1039.2	1045.422559	-0.5987836
9	43	0.632	364	1004.9	1012.338977	-0.740270419
10	42	0.6634	394	1047.2	1041.420014	0.551946715
11	42.2	0.657	380	1025.9	1034.393029	-0.827861311
12	43	0.666	386	1052	1043.251962	0.831562523
13	45	0.6621	382	1044.7	1039.21743	0.524798528
14	45	0.6537	378	1037.2	1030.534511	0.642642615
15	41	0.6617	382	1042.2	1036.387471	0.557717261
16	43.5	0.6652	384	1048.8	1041.515623	0.694543913
17	44	0.6719	388	1053.4	1052.199054	0.11400661
18	42	0.651	376	1024.8	1030.190096	-0.525965652
19	35	0.6518	376	935.6	935.9620754	-0.038699805
20	43.6	0.6442	372	1023.9	1024.175745	-0.026930819
21	46	0.6552	378	1034.6	1028.77706	0.562820403
22	42	0.6556	378	1026.4	1032.464433	-0.590845017
23	44	0.6554	378	1022.7	1031.359338	-0.84671337
24	42.2	0.6594	380	1041.2	1034.708813	0.623433256
25	43	0.6617	382	1045	1037.430826	0.724322853
26	45	0.6552	398	1035.3	1037.562915	-0.218575812
27	49	0.6559	380	1035.1	1034.65861	0.042642293
28	43.5	0.6543	378	1032.8	1031.791281	0.097668352
29	42.9	0.6603	382	1045.2	1037.114844	0.77355111
30	44	0.6536	378	1028.7	1031.482581	-0.270494885
31	40.8	0.6383	368	1012.2	1019.735338	-0.744451482
32	42.2	0.6455	374	1023.2	1027.565596	-0.426661096
33	43	0.6479	374	1026.8	1027.361002	-0.054635981
34	35.1	0.6302	364	937.4	937.1265247	0.029173805
35	42.2	0.6547	378	1033.7	1032.32766	0.132759994
36	32.2	0.6545	378	45.3	45.75856787	-1.012291112
37	56	0.5797	336	933.9	937.3171494	-0.365901
38	53	0.5613	324	910.9	909.9658722	0.102549989
39	54	0.5622	324	905.1	897.6850317	0.819242987
40	29.5	0.6614	382	1049	1041.272041	0.736697753
41	29	0.5636	326	912	905.2306266	0.742255854
42	55	0.5634	326	911.8	912.6598999	-0.094307948
43	49.2	0.5656	326	909.2	923.0698349	-1.525498782

number	Pressure (bar)	Specific Gravity	M_W	NHV (Exp)	NHV (Estimated)	Error (%)
44	51	0.5814	336	937.6	935.2662958	0.248901902
45	26	0.6955	402	1088.6	1094.269494	-0.520805954
46	23.2	0.6598	382	1049.7	1035.520727	1.350792857
47	54	0.5678	328	917	919.191631	-0.23900011
48	26.7	0.5788	334	933	920.7191959	1.316270535
49	56	0.5797	336	933.9	937.3171494	-0.365901
50	54.1	0.5617	324	908.8	900.1197396	0.955134289
51	28	0.5622	324	909.7	916.4244901	-0.739198646
52	28	0.5671	328	916.8	916.5593761	0.026246064
53	53	0.5601	324	908	919.1378767	-1.226638398
54	28.8	0.562	324	909.2	909.267081	-0.007378024
55	45	0.6542	378	1029.1	1030.451379	-0.131316545
56	28.5	0.5608	324	911.5	912.8037094	-0.143029007
57	54.5	0.5607	324	902.6	903.276133	-0.074909481
58	27	0.6898	398	1084	1093.75439	-0.899851467
59	23.2	0.6711	388	1060.9	1062.728337	-0.172338255
60	53	0.5688	328	917	915.4096798	0.173426417
61	52.7	0.5626	324	909.3	901.768102	0.828318268
62	29.5	0.56	324	908.1	890.2303652	1.967804735
63	53	0.6316	366	932.1	924.2497809	0.84220782
64	43	0.5609	324	908.1	910.3094404	-0.243303646
65	51.5	0.6811	392	1052.3	1051.794549	0.048032994
66	24.6	0.6672	386	1058	1062.845042	-0.457943439
67	28	0.5639	326	911	916.4129636	-0.594178218
68	25.3	0.6013	348	950	928.4476459	2.26866885
69	24	0.6717	388	1063.2	1068.312729	-0.480881238
70	28	0.5614	324	910.4	916.3975017	-0.658776553
71	28.1	0.5971	346	923.9	926.2744959	-0.257007894
72	25.3	0.6197	358	930.3	948.6382331	-1.97121714
73	25.2	0.6078	368	926.5	931.0820995	-0.494560116
74	55	0.7586	438	1155	1153.839364	0.100487947
75	54.5	0.6729	390	1045.2	1043.577418	0.15524134
76	54.5	0.6729	390	1045.2	1043.577418	0.15524134
77	56	0.6868	396	907	940.1198133	-3.651578096
78	57	0.6393	370	865	862.6734911	0.268960567
79	57	0.6405	370	825.5	851.7361208	-3.178209664
80	58	0.6439	372	896.2	884.8757338	1.263586941
81	56	0.6889	398	972.9	953.0961468	2.035548685
82	54	0.6437	372	873.1	925.1693038	-5.963727382
83	55	0.6796	392	947.9	975.8686264	-2.950588289
84	54.8	0.7148	414	1029.4	1038.841898	-0.917223424
85	56	0.6402	370	876.5	867.7901719	0.993705434
86	55	0.6418	370	883.6	874.091276	1.076134449
87	55.5	0.6369	368	877.5	859.6428179	2.035006508
88	56	0.6889	398	972.9	953.0961468	2.035548685

V. Results and Discussions

Compared to the development in experimental techniques, the numerical method has been improved. A feed forward back propagation network has been developed as a predicting model of NHV. It was proved that the trained network could well simulate the relation between NHV of crude oil and its properties such as Pressure, specific gravity and molecular weight. The model has been trained, validated and tested on experimental data. The network with one hidden layer shown in Fig. 1 was selected and different neuron in hidden layer was examined. The result of different neuron in hidden layer is shown in Table II.

TABLE II
Result of Neural Networks with Different Neurons in Hidden Layer for Network with one Hidden Layer

Number of neurons in hidden layer	MSE	R^2
1	0.4631	0.5417
2	0.4557	0.5594
3	0.4578	0.7222
4	0.4962	0.9783
5	0.4961	0.9880
6	0.4961	0.9880
7	0.5022	0.9923
8	0.4969	0.9959
9	0.4969	0.9959

According to Table II, the network with 8 neurons in one hidden layer was selected. This network is shown in Fig. 1.

Normalized experimental data versus normalized predicted data by ANN is shown in Fig. 2. And predicted data and its error are shown in last column of Table I.

The training and testing lead to satisfactory results, the network was considered to be well trained and generalized and ready to predict the NHV in other conditions.

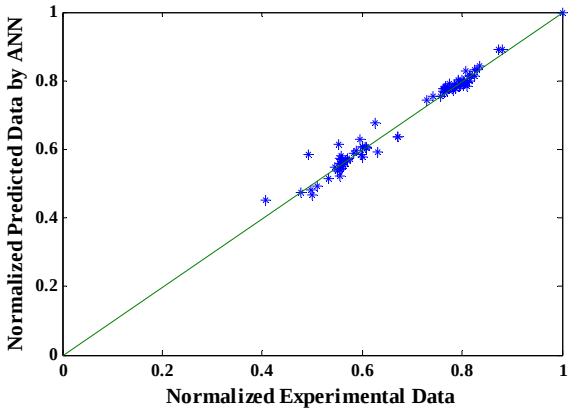

Fig. 2 Experimental and predicted water content in crude oil

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