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Thermal Conductivity Calculation at Moderate Pressure for Polyatomic Gases Using a Neural Network Approach

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Abstract*— The main aim of the present work was the development of a new method based on neural network to accurately evaluate thermal conductivity of pure polyatomic gases included both polar and no polar gases at atmospheric pressure and over wide range of temperature. Two multilayer feed forward neural networks have been trained using five and four physicochemical properties for polar and no polar gases respectively; molecular weight (M), boiling point (T_b), critical temperature (T_c), critical pressure (P_c) and dipole moment (μ), for polar gases, combined with absolute temperature (T) as their inputs . The thermal conductivity and the properties for each individual gas were compiled on different temperatures, ranging from their boiling points to 1100 K. The maximum absolute error in thermal conductivity, predicted by the artificial neural networks ANNs, was less than 4%.

Index Terms*— Conductivity, Polar gases, No polar gases, Artificial neural networks.

I. INTRODUCTION

For the nuclear industry as well as other industries an important aspect is the knowledge and the understanding of the behavior of the fluids particularly the gases in process of heat transfer. The thermal conductivity is indicated as the fundamental property of substances that governs the rate of transfer of heat by conduction. A several methods currently available for gases were proposed by theoretical studies. But none is entirely comprehensive and all have some limitations. On the other hand, an accurate experimental measurement of thermal conductivity of gases, particularly at very high and/or very low temperature, is too laborious and complex task.

At present, the frequently used method is there proposed by Eucken [1], [2] that relate the thermal conductivity (λ) of simple gases to the viscosity (η) and to the heat capacity of pure gases in the ideal-gas state at constant pressure (C^0_p):

$$\lambda = \frac{R}{M}\left[\frac{15}{4} + \left(\frac{C_p^0}{R} - \frac{5}{2}\right)\eta\right] \qquad (1)$$

where R is the perfect gas constant (8.314 J. mol^{-1} .K^{-1}) and M is the molecular weight (g).

There are also some works using ANNs in the prediction of physicochemical properties [3]–[6]. These reports have generally been restricted to liquid rather than gases.

The present work focuses on the development of a thermal gases conductivity model basing on neural networks, which can be applied over wide ranges of temperature and with accurate estimation.

II. PROCEDURE

A. Data base

This study is devoted to polyatomic gases regrouped in the Table I. Because of experimental data insufficiency over wide range of temperature, the thermal conductivities data were completed by (1) and consolidated by some experimental thermal conductivity data [1], [2], [7] every 20 K ranging from their boiling point to 1100 K. The conductivity data obtained for polar and no polar gases have approximately a same size and consist of about 1600 vectors which were divided into two sets and used separately to train and test the ANNs. The training set consist of 70% of data base selected randomly and the remaining vectors, which contained approximately a third of the data base, were used as test set for checking the predictive performance of the ANNs. The variable retained as inputs to the ANNs were absolute temperature and five physical properties (M, T_c, T_b, P_c, and μ) for polar gases and absolute temperature with four physical properties (M, T_c, T_b, and P_c) for non polar gases. They have been selected after exhaustive examination of theoretical models [1], [2].

B. Neural network design

A neural network is a powerful data modelling tool that is able to capture and represent complex input/output relationships. The true power and advantage of neural networks lies in their ability to represent both linear and nonlinear relationships and in their ability to learn these relationships directly from the data being modelled.

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Contrary to the ANN, the traditional linear models are simply inadequate when it comes to modelling data that contains nonlinear characteristics. The AAN are then indicated as universal approximators of complex non-linear relationships between process variables and product quality properties [8], [9]. It has been shown that non-linear feedforward neural networks are capable of universal functional approximation and that a single hidden layer with sigmoid transfer function and one neuron in the output layer with linear transfer function is sufficient to uniformly approximate any continuous bounded function [10].

Table I: List of gases used to provide training and test data of ANNs [1], [2], [7].

Gaz	M, g/mol	T_b, K	T_c, K	P_c, bar	T, K	μ, D	λ, mW/mK
Polar gases							
BrH	80.912	206.43	363.15	85.52	373	0.8	14.5673
CCl_2O	98.916	280.7	455.16	56.74	400	1.1	12.0124
CH_2Cl_2	84.933	313	510	60	500	1.57	22.6435
CH_3Br	94.939	276.71	467.15	52.3	373	1.8	18.2144
CH_3Cl	50.488	249.39	416.25	66.8	373	1.87	12.3024
CH_3F	34.033	194.74	317.7	58.74	420	1.8	19.1623
CH_4O	32.042	337.8	512.6	79.9	400	1.7	9.3264
CH_4S	48.1	279.11	469.95	72.33	380	1.3	7.8796
CH_5N	31.057	266.82	430.05	74.6	420	1.3	15.564
$CHCl_2F$	102.92	282.05	451.65	51.68	460	1.3	16.4812
$CHCl_3$	119.378	334.3	536.4	54	340	1.013	11.8754
CHN	27.026	298.85	456.75	53.9	400	2.7	17.4724
$C_2H_2F_2$	64.027	189.15	302.85	44.63	400	1.4	33.9332
C_2H_3Cl	62.499	259.45	429.65	55.9	340	1.5	32.1183
$C_2H_4F_2$	66.05	248.15	386.65	47.56	340	2.3	72.2321
C_2H_4O	44.053	283.6	468.93	71.91	380	1.9	20.477
C_2H_5Cl	64.514	285.43	460.35	52.66	360	2	27.291
C_2H_5F	48.06	236.05	375.35	50.31	520	2	17.4232
C_2H_5OH	46.069	351.5	516.2	63	500	1.69	22.2241
C_2H_6O	46.069	248.33	400.1	52.69	360	1.3	31.4539
C_2H_7N	45.084	289.75	456.55	56.29	440	1.3	19.6592
C_3H_4	40.065	249.94	402.39	56.28	460	0.7	32.4626
C_3H_6O	58.08	329.4	508.1	46.4	340	2.9	22.0757
CH_3COOCH_3	74.08	330.1	506.8	46.3	380	1.72	23.0644
C_3H_7OH (isopropanol)	60.096	355.4	508.3	47	800	1.69	23.9725
C_3H_7OH (n-propanol)	60.096	370.4	536.7	51	520	1.7	9.7741
C_3H_9N	59.111	276.02	433.3	40.8	360	0.6	18.3265
C_4H_6	54.091	281.23	463.65	47.12	540	0.8	39.2218
$CH_3COOC_2H_5$	88.107	350.3	523.2	37.8	440	1.78	32.5815
$C_4H_{10}O$	74.123	307.7	466.7	35.9	420	1.3	19.4725
COS	60.07	222.92	375	58.77	440	0.7	35.4035
ClH	36.461	188.05	324.55	82.58	323	1.08	38.7982
H_2O	18.015	373.2	647.3	217.6	460	1.85	16.0586
H_2S	34.08	212.95	373.2	89.37	373	0.9	14.0128
H_3N	17.03	239.74	405.55	114.8	280	1.5	22.5538
NOCl	65.459	267.7	440	90	280	1.83	34.4865
O_2S	64.06	263.14	430.8	78.84	360	1.63	101.3752
No polar gases							
BCl_3	117.17	285.65	451.95	38.7	373	0	27.1914
BF_3	67.8	172.85	260.85	49.85	200	0	57.2681
Br_2	159.808	331.9	584.15	103.35	600	0.2	13.5677
CCl_2F_2	120.93	243.37	385.15	41.15	273	0.5	48.5281
CCl_3F	137.38	296.92	471.15	43.74	373	0.5	9.5022
CCl_4	153.823	349.7	556.4	45	300	0	46.5752

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$CClF_3$	104.47	191.65	301.93	38.6	373	0.5	22.234
CF_4	88.01	145.21	227.7	37.43	273	0	229.6003
CH_4	16.043	111.63	190.53	45.96	250	0	11.4232
$C_2Cl_2F_4$	170.93	276.75	418.85	32.63	288	0.5	36.1104
C_2ClF_5	154.48	235.15	353.15	31.6	373	0.3	18.524
C_2F_4	100.016	197.53	306.45	40.5	373	0	42.8193
C_2F_6	138.02	194.95	292.85	29.8	273	0	11.7627
C_2H_2	26.038	189.2	308.33	61.91	198	0	55.9135
C_2H_4	28.054	169.43	282.65	50.76	600	0	137.9663
C_2H_6	30.069	184.47	305.42	48.839	260	0	9.2855
C_2N_2	52.035	252	400.15	59.4	273	0.2	12.561
C_3F_8	188.02	236.45	345.05	26.8	273	0	17.9435
C_3H_4	40.065	238.75	393.85	52.49	273	0.2	15.0277
C_3H_6 (cyclopropane)	42.08	240.35	398.3	55.79	273	0	44.23
C_3H_6 (propylene)	42.08	225.43	364.75	46.1	500	0.4	6.4805
C_3H_8	44.096	231.105	369.82	42.5	600	0	7.7487
C_4F_8	200.04	267.16	388.37	27.77	273	0	13.8793
C_4H_{10} (methylpropane)	58.123	261.45	408.13	37.2	265	0.1	11.093
C_4H_{10} (n-butane)	58.123	272.65	425.18	37.96	600	0	18.41
C_4H_6	54.091	268.65	425.15	43.22	273	0	17.33
C_4H_8 (butene)	56.107	266.9	419.55	39.25	273	0.3	8.2883
C_4H_8 (cis-butene)	56.107	276.87	433.15	42.07	288	0.3	11.59
C_4H_8 (cyclobutane)	56.107	288.66	459.95	49.65	288	0	7.7583
C_4H_8 (methylpropene)	56.107	266.03	417.85	40.01	273	0.5	16.28
C_4H_8 (trns-butene)	56.107	274.03	428.15	40.8	288	0	10.5
C_5H_{12}	72.15	282.65	433.78	31.96	288	0	21.72
C_{l2}	70.906	239.05	417.15	77	600	0.2	13.47
CO	28.01	81.62	132.91	34.987	600	0.1	14.9
CO_2	44.01	194.6	304.28	73.825	200	0	12.72
CS_2	76.131	319.4	552	78	303	0	13.81
D_2	4.029	23.57	38.35	16.65	600	0	11.09
F_2	37.997	84.95	144.3	52.15	373	0	16
B_2F_6	27.67	180.65	289.8	40.53	273	0	13.7
H_2	2.016	20.384	33.24	12.98	200	0	14
HI	127.912	237.75	423.95	83	373	0.5	14.06
N_2	28.0134	77.347	126.2	33.999	600	0	14.2
N_2O	117.17	285.65	451.95	38.7	373	0.4	13.73
NO	67.8	172.85	260.85	49.85	200	0.2	15.61
O_2	159.808	331.9	584.15	103.35	600	0	34.61
SF_6	120.93	243.37	385.15	41.15	273	0	17.7462

The successes of the ANNs depend on the selection of process variables, the quality of the data and are also sensitive to the number of neurons in their hidden layers. Too few neurons can lead to underfitting. Too many neurons can contribute to overfitting. The choice of the number of neurons in the hidden layers is therefore, a delicate compromise between providing sufficient neurons to adequately determine an approximate functional relationship, and avoiding the use of too many neurons which can lead to overfitting.

After the examination of a considerable number of differently structured neural networks, the adequate ANNs selected in this investigation had a single hidden layer with 35 neuron for polar gases and 30 neuron for no polar gases and an output layer with one neuron. The hidden layer had a logsig and tansig transfer function for polar and no polar gases respectively. The output layer had a purelin transfer function. Fig. 1 shows the typical structure of an artificial neural network (case of polar gases). The neurons are represented by a circle. Each neuron in the hidden layer receives weighted inputs plus bias from each input (input layer) and as the same output neuron receives weighted inputs plus bias from each neuron in the hidden layer.

Equation (2) formulate the thermal conductivity estimated by the designed ANN, where *Xj* represents the inputs variables (T, M, T_c, T_b, P_c, and μ) and *Wij* being the weights from input (j) to neuron (i) with b_i and b_{36} representing bias of the neurons in hidden layer and bias of the neuron in output layer, respectively.

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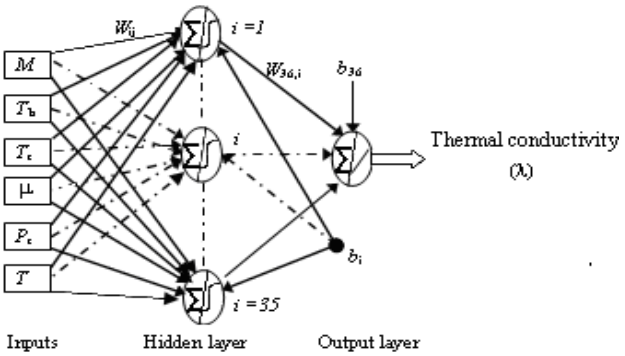

Fig.1: Schematic operation of the ANN

$$\lambda = \sum_{i=1}^{35} W_{36,i} \left\{ \frac{1}{1+\exp\left(-\left(\sum_{j=1}^{6} W_{i,j} X_j + b_i\right)\right)} \right\} + b_{36} \qquad (2)$$

C. Normalization

The normalisation of data values is crucial step in the conception of the ANNs. Almost values of the physical input properties to the ANN differed by several orders of magnitude, which may not reflect the relative importance of the properties in determining thermal conductivity, the entire inputs matrix variables (X_j) , for both polar and non polar gases, were normalized by using the following expression:

$$X_j^N = \frac{X_j}{\left(\sum_{j=1}^{n} X_j^2\right)^{1/2}} \qquad (3)$$

where X_j^N are the re-scaled input values and $n=1,...,6$ labels the input patterns (case of polar gases). However, the target thermal conductivity values were not different by important orders of magnitude so there was not a need to be normalized.

III. RESULTS AND ANALYSIS

We have realised this study with the commercially available neural network toolbox supplied for the Matlab package due to its flexibility. The training algorithm used was "trainlm" which includes Lavenberg-Marquadt back propagation. To prevent over training, we have chosen to train the ANNs until the minimum of the mean of squared errors (MSE) performance function.

Table II summarizes the statistical performance of the designed ANNs. These statistical parameters were calculated from expressions given in a previous work [8], for both training and test (predicted) sets.

Table II: Statistical performance of the trained ANNs for gas thermal conductivity

Property	**Correlated**	**Predicted**
Polar gases		
Squared Correlation Coefficient (*R*)	0.9999	0.9999
Root-Mean-Square Error *(RMSE)*	0.1077	0.1161
Average Absolute Error (*AAE*)	0.147%	0.191%
Standard Deviation *(STDEV)*	0.246%	0.386%
Absolute Error (AE_{max})	3.042%	3.295%
No polar gases		
Squared Correlation Coefficient (*R*)	0.9999	0.9999
Root-Mean-Square Error *(RMSE)*	0.1560	0.1994
Average Absolute Error (*AAE*)	0.40%	0.41%
Standard Deviation *(STDEV)*	0.530%	0.584%
Absolute Error (AE_{max})	3.63%	3.81%

The results obtained by the designed ANNs were represented in the Table III. These were compared with experimental thermal conductivities and with the theoretical models. The average absolute error for the estimated thermal conductivity by the designed ANNs is 0.95% for polar gases and 1.28% for no polar gases (see Table III), according to the experimental thermal conductivity, for a simple of gases, at various temperatures. However, the AAE of other models, are all greater than the AAE value of the ANNs.

An additional other tests consisting of an experimental sample was also effectuated in order to verify the performances of the designed ANNs. The results are given by the Fig. 2 and Fig. 3. The average absolute error is less than 2.5% case of polar gases and less than 1.40% case of no polar gases as indicated in Fig. 2 and Fig. 3.

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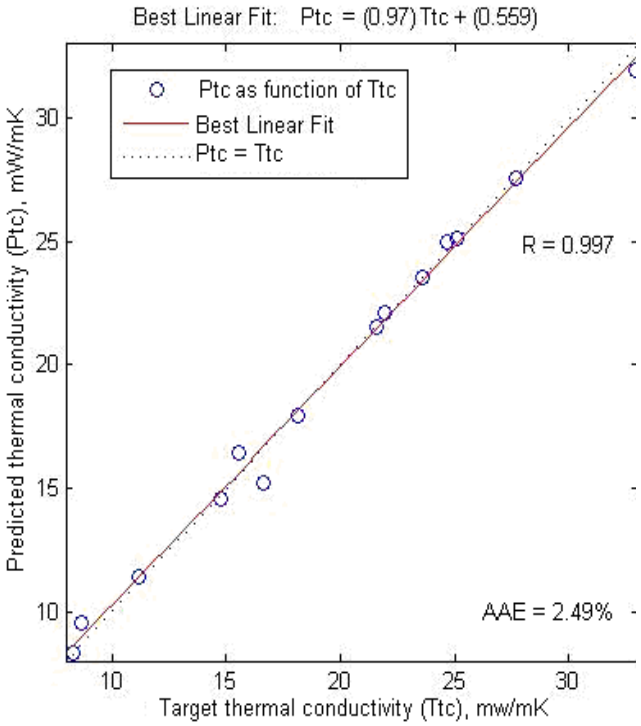

Fig. 2: Predicted results (polar gases)

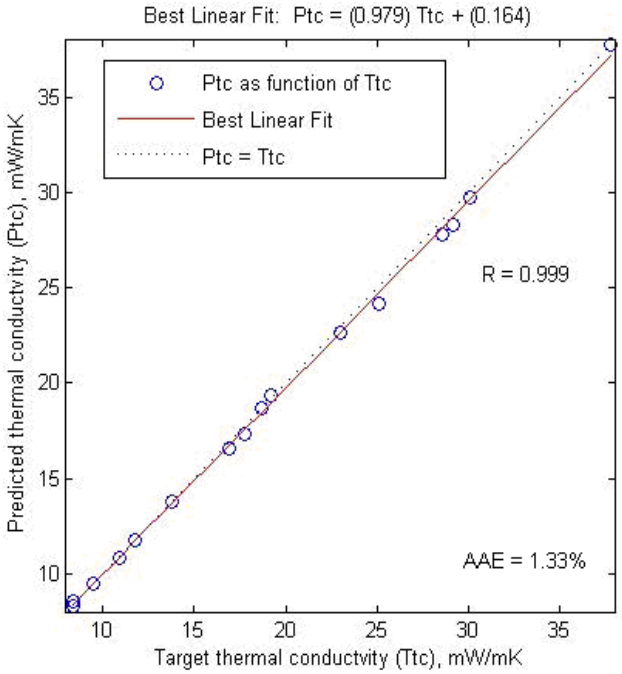

Fig. 3: Predicted results (no polar gases)

IV. CONCLUSION

The value of using ANNs to correlate and predict the polyatomic gases thermal conductivity at moderate pressure (about 1 bar), over wide range of temperature has been demonstrated. Indeed, when the predicted values of polar and no polar gases (Fig. 2, Fig. 3, and Table III) are considered jointly the AAE is approximately 1.51% and the maximum absolute error in thermal conductivity, predicted by the artificial neural networks ANNs, was less

Table III: Comparison between ANNs and theoretical models according to the experimental values of low-pressure gas thermal conductivity

Compound	T, K	Experimental value, mW/mK[1]	Absolute error [(calc. – exp.)/exp.]*100, %									
			Eucken[1]		Modified Eucken[1]		Bromley[1]		Roy-Thodos[1]		Proposed ANN	
			λ	AE	λ	AE	λ	AE	λ	AE	λ	AE
Polar gases												
Acetone	300	11.38	11.40	0.2	13.66	20	12.39	8.9	12.05	5.9	11.19	1.76
	340	14.57	15.15	4.0	17.05	17	15.58	6.9	15.07	3.4	14.73	1.11
	380	17.92	19.00	6.0	20.61	15	19.07	6.4	18.30	2.1	18.16	1.34
	420	21.52	23.24	8.0	24.32	13	22.79	5.9	22.04	2.4	21.58	0.31
	460	25.12	27.26	8.5	28.13	12	26.70	6.3	26.10	3.9	25.08	0.14
Ammonia	273	22.14	24.18	9.2	26.57	20	23.07	4.2	-	-	21.93	0.97
	373	31.98	36.78	15	41.25	29	34.28	7.2	-	-	32.90	2.86
Isopropyl alcohol	400	24.99	28.99	16	25.99	4.0	25.99	4.0	25.29	1.2	24.65	1.36
Water	373	23.57	30.17	28	33.00	40	25.53	8.3	-	-	23.58	0.05
	413	26.58	32.69	23	35.88	35	29.05	9.3	-	-	27.68	0.35
Sulfur dioxide	273	8.29	9.00	8.6	10.03	21	9.37	13	-	-	8.27	0.22
AAE, %				11.5		20.54		7.31		3.15		0.95
No polar gases												
Acetylene	198	11.76	12.24	4.1	13.52	15	11.97	1.8	12.94	10	11.76	0.00

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	273	18.67	19.23	3	21.66	16	20.07	7.5	19.73	5.7	18.74	0.38
	323	24.20	24.44	1	27.35	13	25.60	5.8	24.85	2.7	25.07	3.63
	373	29.76	30.89	3.8	33.03	11	30.92	3.9	30.33	1.9	30.07	1.02
Carbon dioxide	200	9.50	10.01	5.4	10.93	15	10.02	5.5	-	-	9.55	0.47
	300	16.66	17.14	2.9	17.98	7.9	16.96	1.8	-	-	16.90	1.43
	473	28.34	28.94	2.1	31.46	11	30.27	6.8	-	-	29.23	3.15
	598	37.84	39.66	4.8	41.40	9.4	39.66	4.8	-	-	37.82	0.05
Carbon tetrachloride	273	5.94	6.49	9.3	6.52	9.8	6.05	1.9	6.51	9.6	8.41	1.98
	373	8.58	9.05	5.5	9.89	15.3	9.37	9.2	9.06	5.6	9.19	0.18
	457	10.88	11.45	5.2	12.62	16	12.08	11	12.73	17	10.86	0.21
Dichlorodifluoro mathane	273	8.29	9.37	13	8.60	3.7	8.53	2.9	8.35	0.7	8.37	0.96
	373	13.81	16.30	18	14.04	1.7	14.67	6.2	13.87	0.4	13.82	0.03
	473	19.38	23.45	21	20.12	3.8	20.45	5.5	20.12	3.8	19.15	1.18
Ethylene	273	17.37	17.46	0.5	19.45	12	18.06	4	17.42	0.3	17.80	2.48
	323	22.65	23.08	1.9	25.37	12	23.90	5.5	22.70	0.2	23.03	1.70
	373	27.84	28.23	1.4	31.74	14	30.21	8.5	28.68	3	28.63	2.85
AAE, %				6.05		10.97		5.45		4.68		1.28

[1] Values were obtained from [1].

than 4%. These show that the ANNs can be seriously competed the commonly used methods. On the other hand, this method can be applied without depending on many complicated parameters like heat capacity, molecular diameter (σ), acentric factor (ω), energy-potential parameter (ε) and collision integral (Ω_v), that are used in the almost other methods.

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