One parameter Viscosity-Temperature Correlation for Homologous n-Alkanes Series from CH_4 to $C_{20}H_{42}$

Harith Hasoon Jasim / M.Sc. in Chemical Engineering
Lectural Ass. / College of Engineering / Material Dept.
Al-Mustansiriya University
E-mail: eng.harithjasim@yahoo.com

Abstract

The main aim of this paper is to establish a correlation for prediction the dynamic viscosity of homologous n-alkanes from CH_4 to $C_{20}H_{42}$ at isobaric condition within a given temperature range. In this paper, new empirical correlation for dynamic viscosity is generalized as a function of carbon number and temperature. The mean average absolute deviation between the experimental data [13] and the empirical correlation is 2.8411% for 97 data points. These values showing that the statistical analysis model is stable and can be used to obtain good predictions for the same components in a wider range of temperature and for compounds that were not used in the model calibration.

Keywords: n-alkanes, viscosity, carbon number, correlation, homologous

ايجاد معادلة اللزوجة ـ كدالة لدرجة الحرارة ـ ذات العامل الاحادي لحساب لزوجة الالكانات المتسلسلة من CH_4 الى $C_{20}H_{42}$

الخلاصة

الهدف من هذا البحث هو ايجاد علاقة لايجاد قيمة تقريبية للزوجة الديناميكية للالكانات من CH_4 الى $C_{20}H_{42}$ ضمن مدى درجات حرارة معينة في ضغط متساوي. في هذا البحث تم ايجاد معادلة تجريبية جديدة لقياس اللزوجة الديناميكية اعتمادا على درجة الحرارة وعدد ذرات الكاربون لكل مركب من الالكانات. معدل الانحراف بين القيم التجريبية [13] والمعادلة التجريبية كانت 2,8411% لخمسة وتسعون قيمة. تبين ان التحليل الاحصائي ثابت ويمكن استخدامة للحصول على تكهنات لمدى اوسع من درجات الحرارة وتكهنات لباقي المركبات غير المدرجة.

Introduction

Viscosity is a measure of the resistance of a fluid which is being deformed by either shear stress or tensile stress. Viscosity describes a fluid's internal resistance to flow and may be

thought of as a measure of fluid friction. The liquid viscosity of organic compounds is an important property for the simulation of the processes in chemical and petroleum industries.[1,2]

The viscosities of liquids decrease with increasing temperature either under isobaric or as saturated liquids. For a temperature range from the freezing point to somewhere around the normal boiling temperature, it results good approximation when assume ln η_L is linear in reciprocal absolute temperature. [3]

The importance of liquid viscosity in chemical process engineering design makes it one of the most measured transport properties. Liquid viscosity has a direct and large effect on heat transfer coefficients, which are especially important for heat exchangers and various other heat transfer considerations, and are also somewhat important in distillation calculations. Viscosity data are also essential for calculating pressure drops, as for pump and piping calculations. [4]

Recent accurate experimental measurements by different techniques of the viscosity of certain n-alkanes have shown that even for common member of this series, the American Petroleum Institute Tables (71 API) are in error by up to 3% at temperatures not far removed from room temperature. [5, 6]

While many prediction methods for the n-alkane viscosity (η) have been developed over the years, Poling, Prausnitz, and O'Connell [7] point out that "little theory has been shown to be applicable to estimating liquid viscosities". Therefore, most estimation methods are empirical in nature. They have found that often these methods fail significantly, particularly near the normal boiling point. Moreover, experimental data measured at lower temperatures are often extrapolated to higher temperatures with erroneous results.

Sastri and Rao developed a new method for estimating liquid viscosity versus temperature, a method which is based in part on a group contribution method for estimating η. With only minor additional effort, one could use the η-predicting part of the Sastri-Rao method as a means of refining the range of the presently proposed empirical rule for a particular compound of interest. [8]

A viscosity-temperature equation and corresponding chart had beed developed by Christopher J. Seeton to extend the range of ASTM viscosity-temperature charts. The new chart and equation extends the temperature and viscosity range for hydrocarbons and, for the first time, has the ability to extend to the low viscosity regime of halocarbons and low temperature fluids. The new equation and chart can linearize liquid viscosity date from 0.04 cSt and covers the temperature range from -210 to 500°C for halocarbons and hydrocarbons. [9]

A kinematic viscosity–temperature correlation for liquid petroleum fractions has been developed by S. I. Abu-Eishah to represent the experimental data for a wide range of temperatures (100 to 400°F, 37.8 to 204.4°C). The only characterization properties required for estimation are the API gravity and the 50% boiling-point temperature. Fitting parameters have been evaluated for 156 experimental data points from 12 true boiling-point fractions of Arab heavy, Arab medium, and Arab Berri (extralight) crude oils with boiling ranges from

200 to 850°F (93.3 to 454.4°C) and also for 102 data points of 34 other world crude oil fractions. In addition, fitting parameters have also been evaluated for both Arabian and other world crude-oil fractions. The proposed correlation fits the kinematic viscosity data with an overall average relative error of 2.75% for the 12 Arabian crude-oil fractions and 4.46% for the 34 other world fractions. The fitting correlation when used for all available experimental data gives an overall average error of only 3.5%. [10]

New correlations to predict natural gas viscosity was developed by Ehsan Heidaryan, Jamshid Moghadasi and Masoud Rahimi. The study proposed two new accurate simple explicit numerical methods for calculating the viscosity of natural gases. Results of these correlations are compared versus experimental data. The output of this correlation can be directly assumed or be used as an initial value of other implicit correlations. In addition, this correlation is valid for gas coefficient of isothermal compressibility calculations. [11]

A method based on the effective carbon number is presented by Juliet Mcclatchey Allan, Amyn S. Teja for the correlation and prediction of the viscosity of liquid hydrocarbons and hydrocarbon mixtures. It is proposed that the effective carbon number for the substance of interest be obtained from a single viscosity datum in the liquid range. The viscosity-temperature relationships of sixty-nine hydrocarbons, eleven defined hydrocarbon mixtures and eight crude oil fractions were studied in the present work. In general, calculated viscosities compared favorably with experimental data for all the systems studied. [12]

New Correlation Development

In order to obtain the most satisfactory representation of the temperature and the number of carbon atoms dependence of the n-alkane viscosities, attention was paid to the need for the expression to fit the selected data based on laboratory experimental of viscosity measurement for n-alkanes from methane (CH_4) to n-Eicosane ($C_{20}H_{42}$) in liquid state by Reid, Prausnitz and Sherwood [13]. Statistica (v.7) used to generate below correlation and the constants A1 to D5. This correlation gives a functional relationship between the alkane's viscosity with the corresponding temperature and carbon numbers. The correlation obtained is:

$$\eta_c = A_1 + A_2C + A_3(C+20/T)^{A_4} + (B_1C^{B_2}T^{B_3}(C+20/T)^{B_4})(D_1 + D_2T + D_3C + D_4(C+200/T)^{D_5})^{D_4} \quad ....(1)$$

The equation constants are shown in Table 1.
Where:
η = viscosity of n-alkane, cP
T = temperature, K
C = number of carbon atoms of the n-alkane component
A1, A2, A3, A4, B1, B2, B3, B4, D1, D2, D3, D4, D5 = constants of Eq.1

Table 1: Constants of Eq.1

Constant	Value
A_1	0.146380
A_2	0.009482
A_3	-0.069491
A_4	0.381330
B_1	0.096133
B_2	4.799001
B_3	9.593554
B_4	-4.43083
D_1	28.47569
D_2	0.232535
D_3	1.701606
D_4	-12.8457
D_5	0.583917

Discussion

This correlation has been found to be remarkably powerful in practice, providing a valuable link between the regression, extrapolation, prediction, and evaluation viscosity at a wider range of temperature. The temperature range application of the proposed correlation (Eq.1) is shown in Table (2). Also, an interesting overall trend of viscosity values decreasing with increasing carbon number within the studied compounds has been observed.

An analysis for application of the proposed formula (Eq.1) has been made, where the overall absolute average percentage error is 2.8411 % for 97 data points. Table (3) demonstrates the percentage error between measured and calculated viscosity values. Figure (1) shows a comparison between the measured values of viscosity and the predicted values according to the aforementioned generalized correlation. Figure (2) shows the fluctuated percent error (calculated by Eq.1) for all the available n-alkanes viscosity data along with number of carbon atoms for n-alkanes components. Figure (3) shows the fluctuated absolute percent error for each n-alkanes component. It's found that the error between the measured and calculated viscosity decreases with increasing the number of carbon atoms and slightly increased in n-Octadecane, n-Nondecane and n-Eicosane components. Figure (4) to Figure (23) show the graphical representation of the measured viscosity values with the corresponding calculated ones.

Conclusion

The dynamic viscosity for n-Alkanes from Methane to n-Eicosane can be calculated theoretically by using equation (1). The overall error will be 2.8411 %. The error for the first four components (From Mehtane CH_4 to n-Eiconsane $C_{20}H_{22}$ will be 5.825% then the error will decrease to 2.169% for the rest components.

Nomenclature

η: Viscosity of n-alkane, cP

η_{Ib}:   Viscosity at normal boiling point, cP

T: Temperature, K

C: Number of carbon atoms for n-alkene component

A1, A2, A3, A4, B1, B2, B3, B4, D1, D2, D3, D4, D5:   Constants of Eq.1

% E: Percentage error

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Table 2: The temperature range of the application proposed Correlation (Eq.1)

Component	Formula	Temperature range, oC	
		Min.	Max.
Methane	CH_4	-180	-84
Ethane	C_2H_6	-183	32
Propane	C_3H_8	-187	96
n-Butane	C_4H_{10}	-90	0
n-Pentane	C_5H_{12}	-130	40
n-Hexane	C_6H_{14}	-95	70
n-Heptane	C_7H_{16}	-90	100
n-Octane	C_8H_{18}	-55	125
n-Nonane	C_9H_{20}	-50	150
n-Decane	$C_{10}H_{22}$	-25	175
n-Undecane	$C_{11}H_{24}$	-25	200
n-Dodecane	$C_{12}H_{26}$	-5	220
n-Tridecane	$C_{13}H_{28}$	-5	240
n-Tetradecane	$C_{14}H_{30}$	5	255
n-Pentadecane	$C_{15}H_{32}$	10	280
n-Hexadecane	$C_{16}H_{34}$	20	280
n-Heptadecane	$C_{17}H_{36}$	25	200
n-Octadecane	$C_{18}H_{38}$	30	300
n-Nondecane	$C_{19}H_{40}$	35	300
n-Eicosane	$C_{20}H_{42}$	40	300

Table 3: Comparisons of measured and calculated viscosity values at different temperatures

n-alkane components	Temperature,°K	Measured Viscosity [13], cP	Calculated Viscosity, cP	% Error
Methane	93.150	0.21	0.227	-8.095
	117.150	0.131	0.143	-9.160
	141.150	0.112	0.12	-7.143
	165.150	0.121	0.11	9.091
Ethane	90.150	1.426	1.442	-1.122
	142.150	0.271	0.241	11.070
	197.150	0.146	0.142	2.740
	251.150	0.094	0.113	-20.213
Propane	86.150	10.182	10.175	0.069
	156.150	0.471	0.432	8.280
	227.150	0.205	0.181	11.707
	298.150	0.112	0.122	-8.929
n-Butane	183.150	0.609	0.532	12.644
	205.150	0.403	0.376	6.700
	228.150	0.32	0.282	11.875
	250.150	0.253	0.227	10.277
	273.150	0.206	0.188	8.738
n-Pentane	143.150	2.966	3.092	-4.248
	185.150	0.944	0.948	-0.424
	228.150	0.453	0.45	0.662
	270.150	0.277	0.275	0.722
	313.150	0.192	0.193	-0.521
n-Hexane	178.150	1.926	2.018	-4.777
	219.150	0.801	0.824	-2.871
	260.150	0.439	0.445	-1.367
	302.150	0.281	0.281	0.000
	343.150	0.202	0.202	0.000
n-Heptane	183.150	3.215	3.042	5.381
	230.150	1.047	1.041	0.573
	278.150	0.493	0.499	-1.217
	326.150	0.289	0.297	-2.768
	373.150	0.196	0.205	-4.592

	218.150	1.951	1.99	-1.999
	263.150	0.829	0.854	-3.016
n-Octane	308.150	0.453	0.464	-2.428
	353.150	0.288	0.295	-2.431
	398.150	0.203	0.211	-3.941
	223.150	2.652	2.6	1.961
	273.150	0.983	0.99	-0.712
n-Nonane	323.150	0.495	0.501	-1.212
	373.150	0.3	0.305	-1.667
	423.150	0.204	0.212	-3.922
	248.150	2.059	2.095	-1.748
	298.150	0.864	0.88	-1.852
n-Decane	348.150	0.465	0.47	-1.075
	398.150	0.292	0.296	-1.370
	448.150	0.204	0.21	-2.941
	248.150	2.848	2.8	1.685
	304.150	1.012	1.016	-0.395
n-Undecane	361.150	0.491	0.494	-0.611
	417.150	0.293	0.298	-1.706
	473.150	0.197	0.207	-5.076
	268.150	2.364	2.387	-0.973
	324.150	0.926	0.935	-0.972
n-Dodecane	380.650	0.476	0.477	-0.210
	437.150	0.291	0.294	-1.031
	493.150	0.199	0.208	-4.523
	268.150	2.995	3.005	-0.334
	329.150	1.041	1.046	-0.480
n-Tridecane	391.150	0.499	0.498	0.200
	452.150	0.294	0.298	-1.361
	513.150	0.197	0.208	-5.584
	278.150	2.987	3.013	-0.870
	341.150	1.041	1.043	-0.192
n-Tetradecane	403.150	0.509	0.506	0.589
	466.150	0.299	0.302	-1.003
	528.150	0.2	0.212	-6.000
	283.150	3.298	3.285	0.394
	350.150	1.079	1.069	0.927
n-Pentadecane	418.150	0.5	0.494	1.200
	486.150	0.288	0.291	-1.042

	553.150	0.191	0.205	-7.330
n-Hexadecane	293.150	3.177	3.183	-0.189
	358.150	1.109	1.097	1.082
	423.150	0.535	0.525	1.869
	488.150	0.313	0.315	-0.639
	553.150	0.208	0.221	-6.250
n-Heptadecane	298.150	3.356	3.359	-0.089
	342.150	1.581	1.565	1.012
	386.150	0.884	0.865	2.149
	430.150	0.557	0.543	2.513
	473.150	0.385	0.38	1.299
n-Octadecane	303.150	3.356	3.496	-4.172
	371.150	1.138	1.162	-2.109
	438.150	0.544	0.552	-1.471
	506.150	0.314	0.328	-4.459
	573.150	0.208	0.232	-11.538
n-Nondecane	308.150	3.618	3.595	0.636
	374.150	1.271	1.235	2.832
	441.150	0.606	0.583	3.795
	507.150	0.353	0.35	0.850
	573.150	0.233	0.247	-6.009
n-Eicosane	313.150	3.722	3.657	1.746
	378.150	1.335	1.284	3.820
	443.150	0.647	0.618	4.482
	508.150	0.377	0.372	1.326
	573.150	0.249	0.262	-5.221
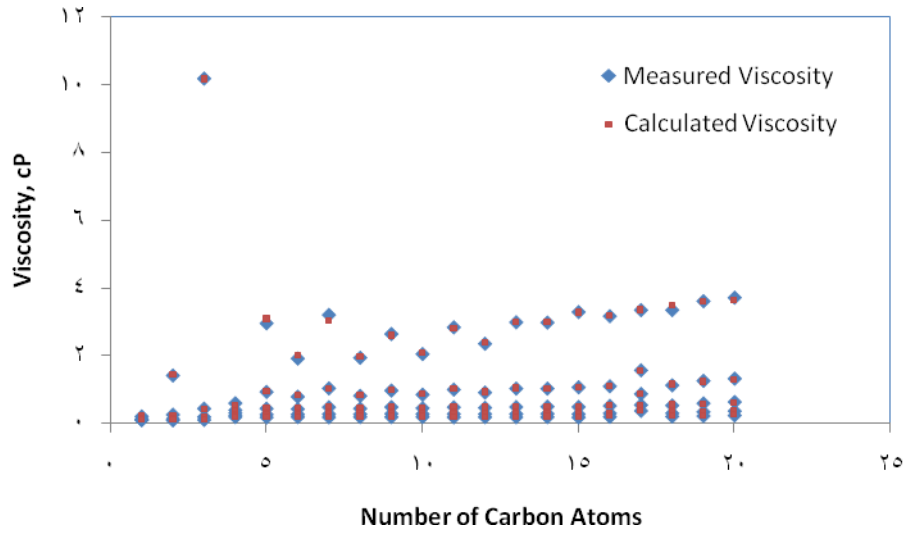
Figure 1: Comparisons between measured values and predicted viscosity values with the number of carbon atoms for each component.
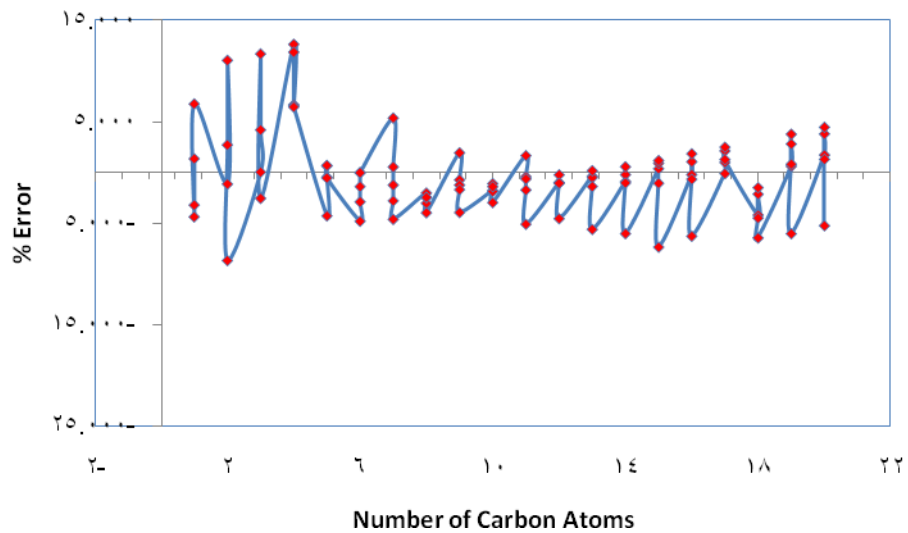
Figure 2: Percent error of calculated viscosity of n-alkanes.
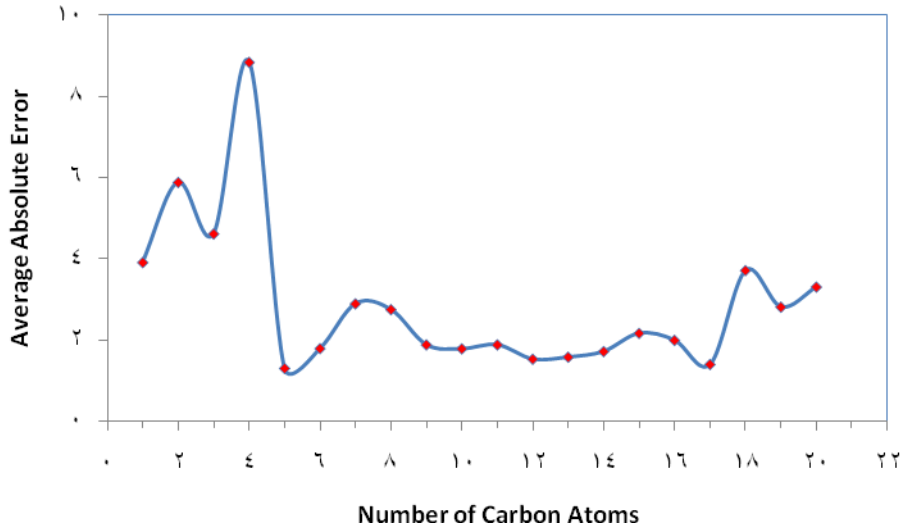
*Figure 3: Average Absolute Percent Error of Calculated Viscosity Of Each N-Alkane Component.*
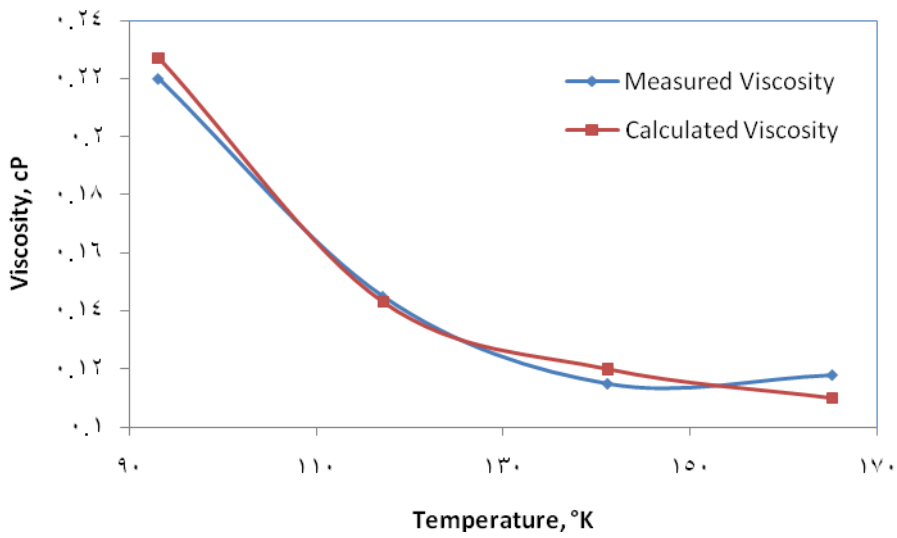
Figure 4: Comparison between measured and calculated viscosity for Methane.

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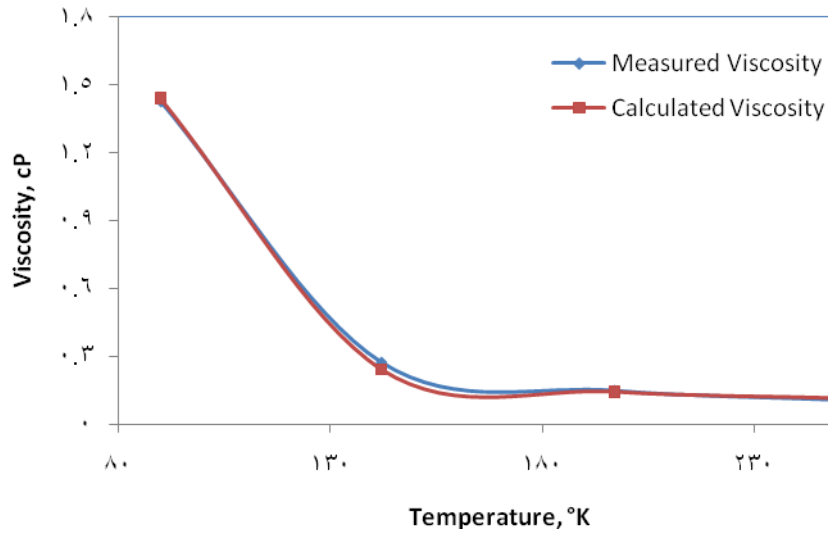
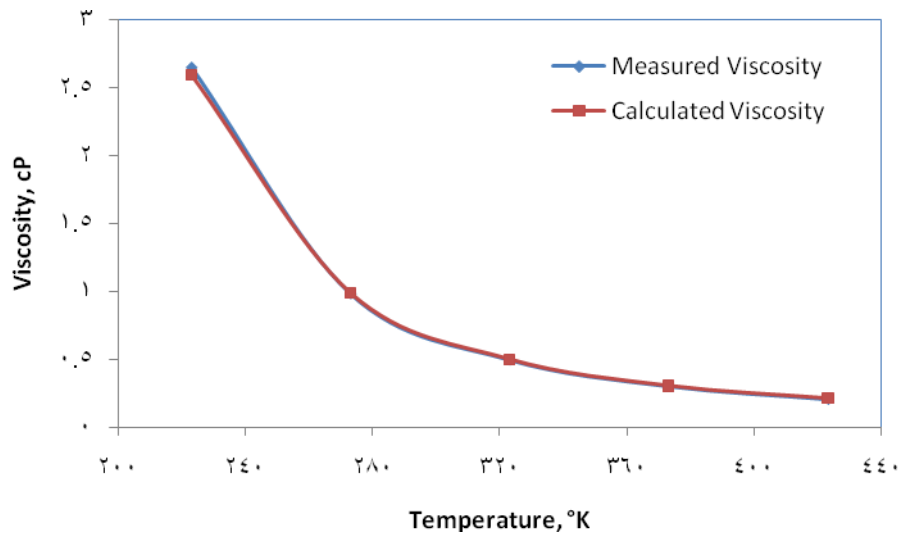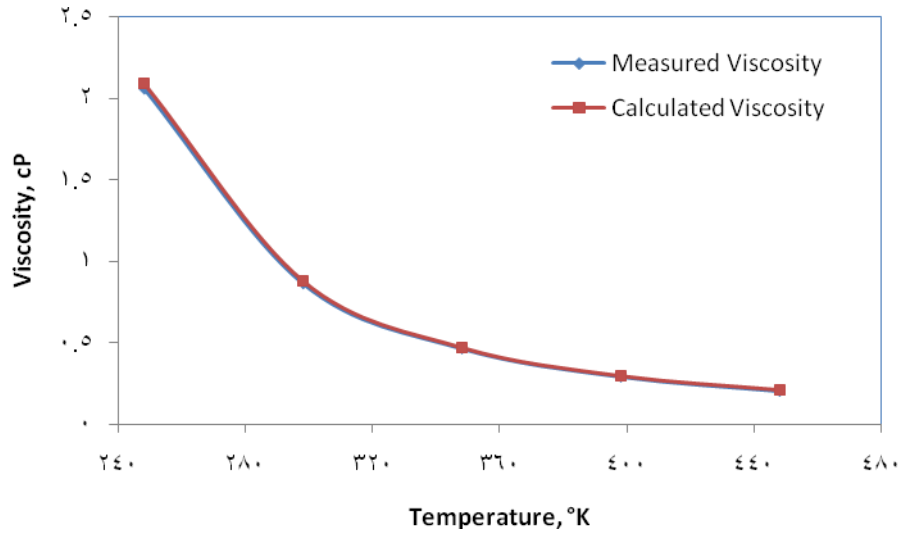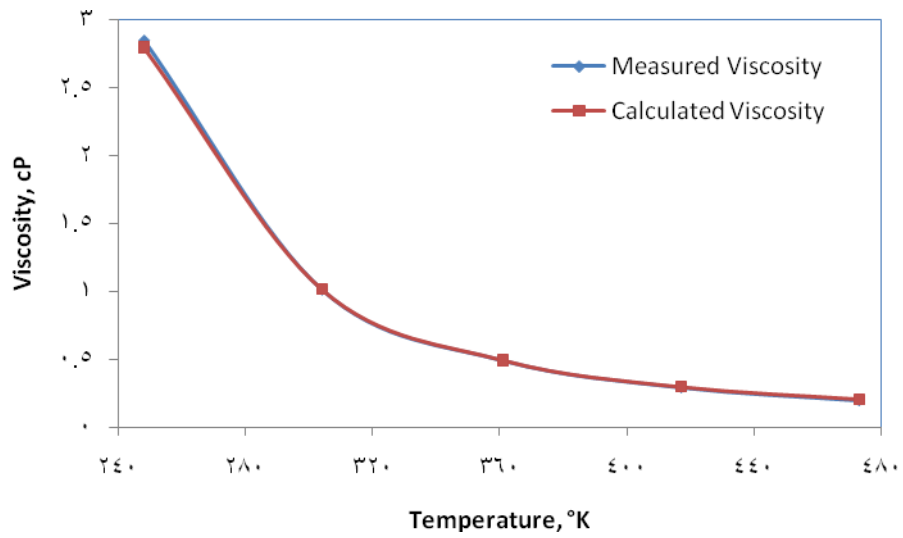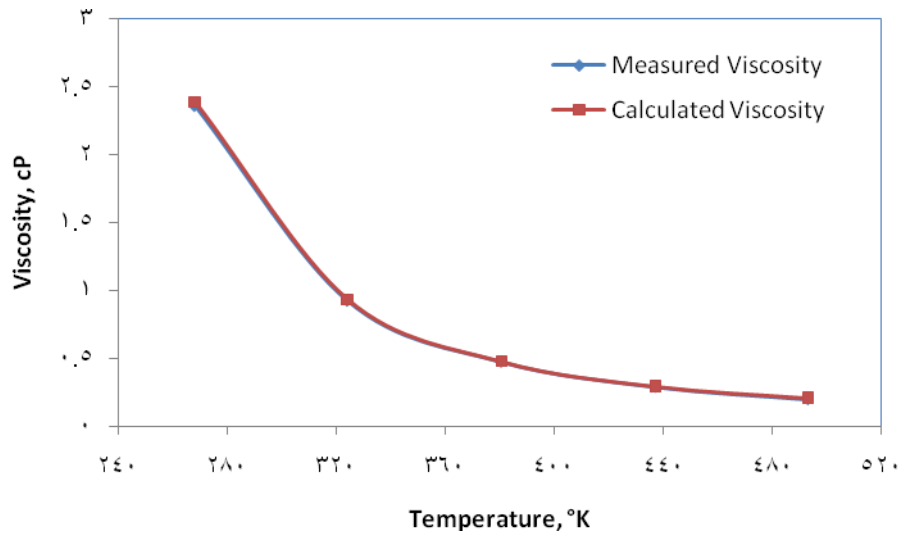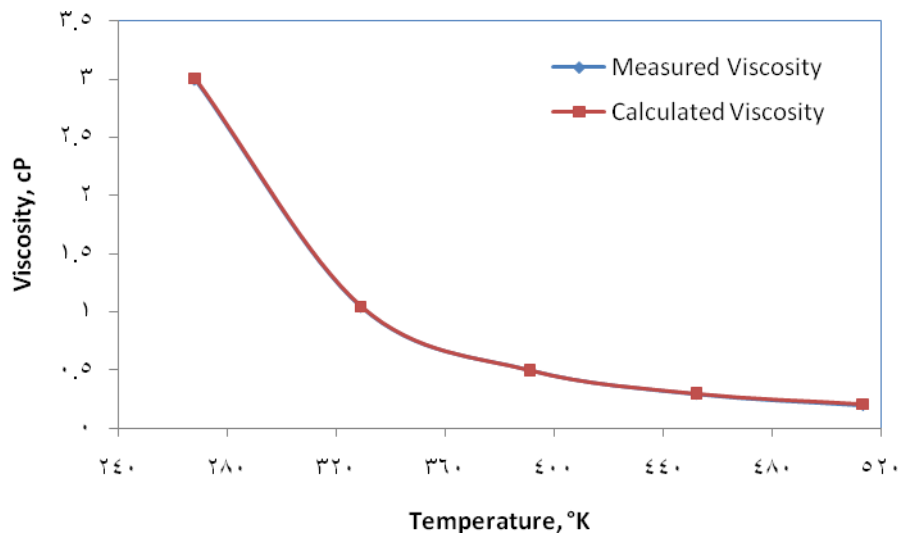*Figure 5: Comparison between measured and calculated viscosity for Ethane.*
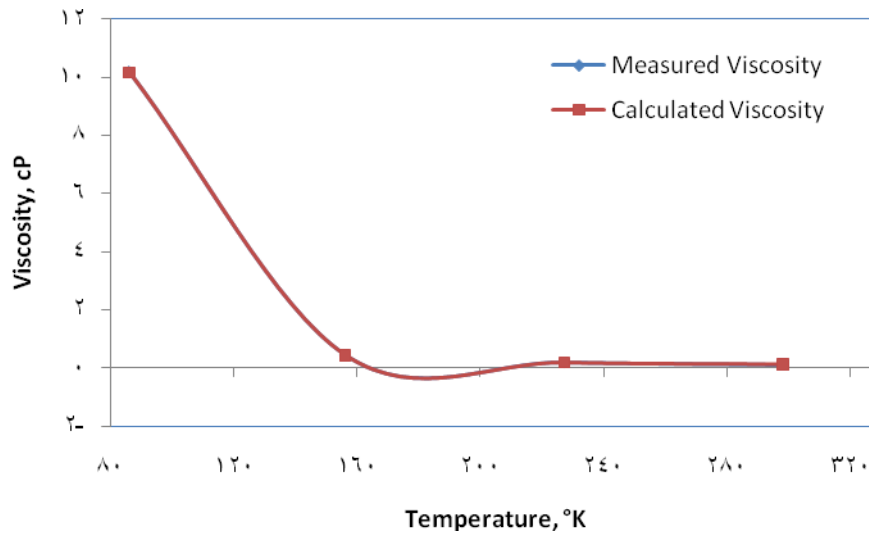
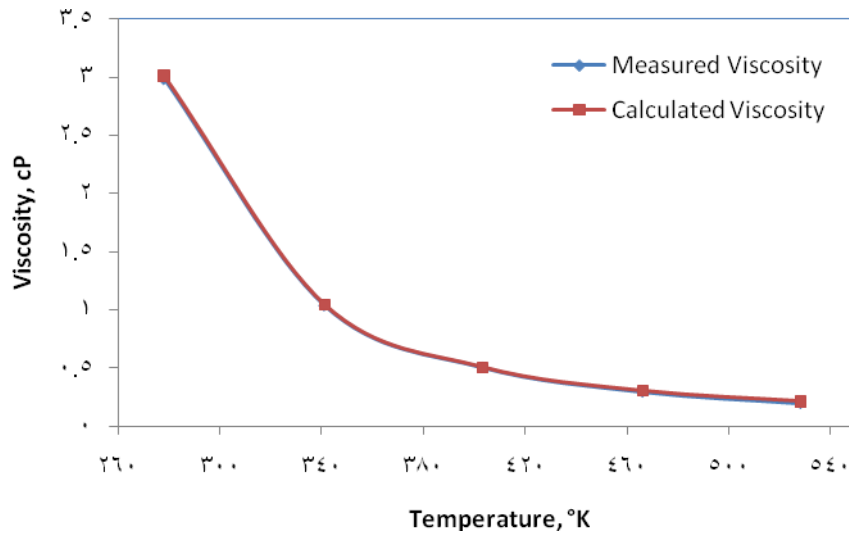*Figure 6: Comparison between measured and calculated viscosity for Propane.*
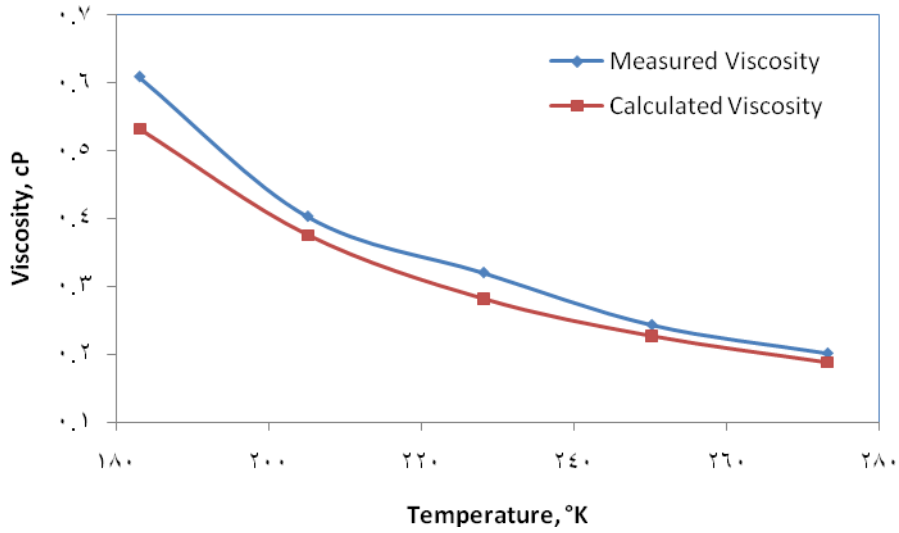
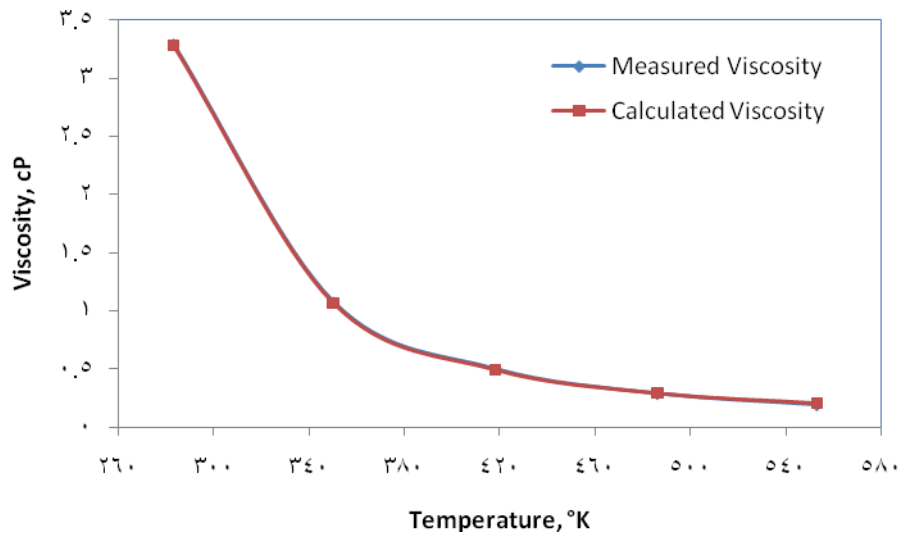***Figure 7: Comparison between measured and calculated viscosity for n-Butane.***
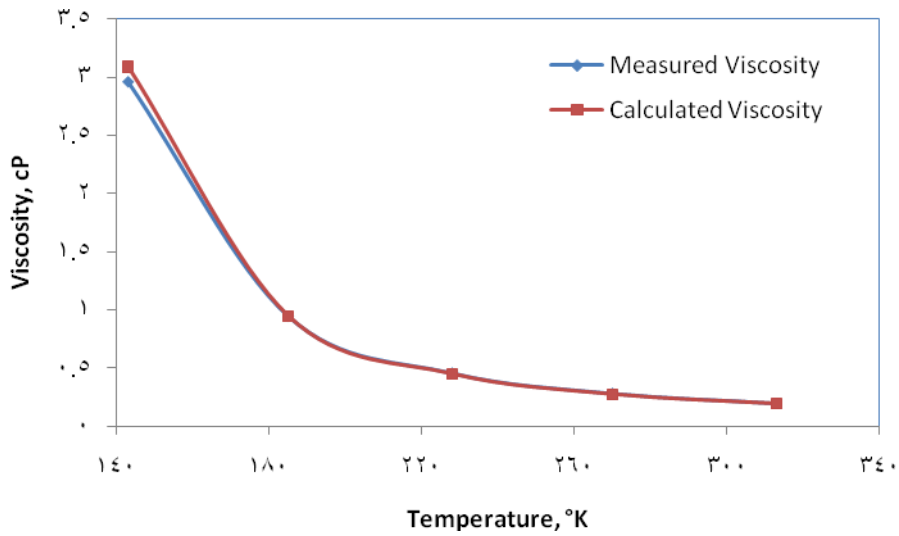
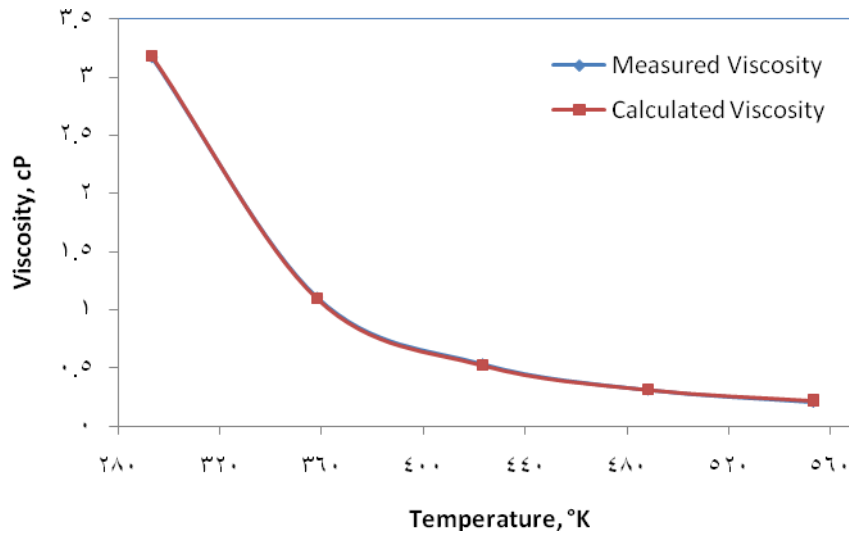***Figure 8: Comparison between measured and calculated viscosity for n-Pentane.***
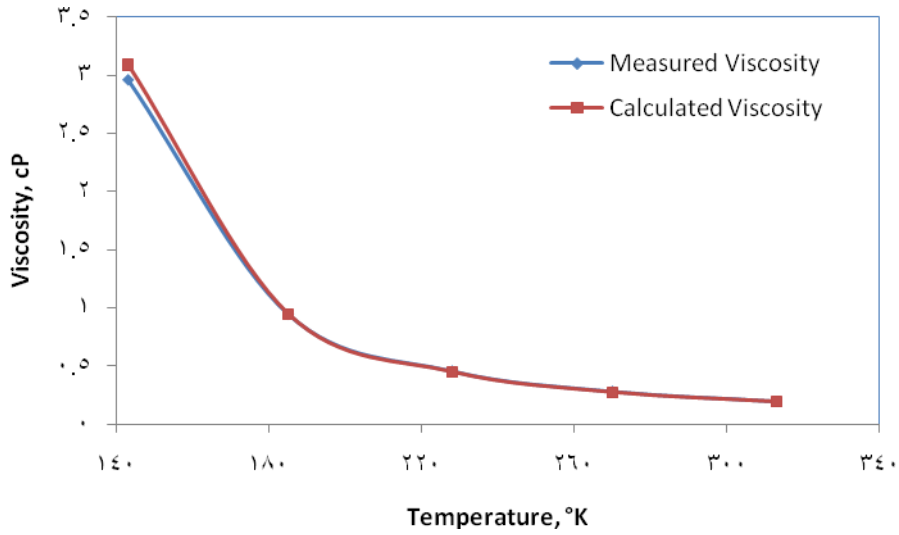
Figure 9: Comparison between measured and calculated viscosity for n-Hexane.
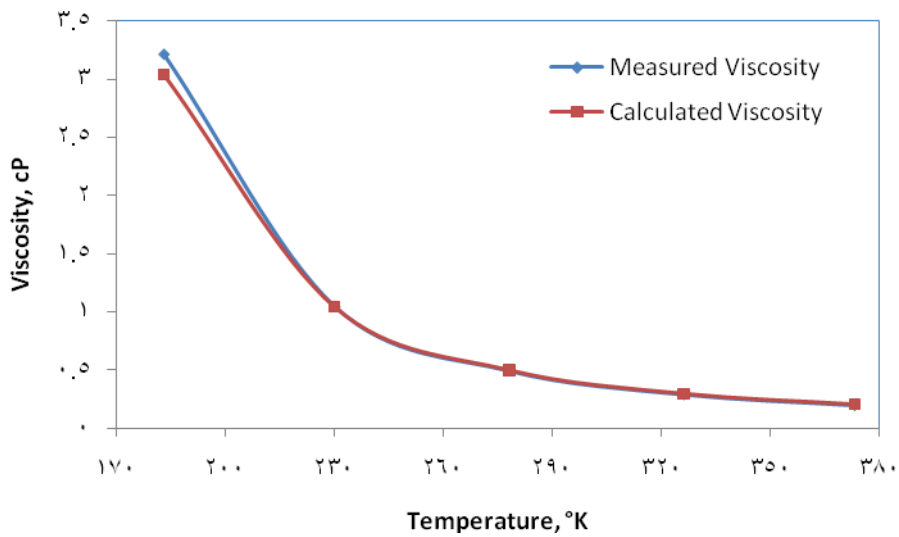
Figure 10: Comparison between measured and calculated viscosity for n-Heptane.
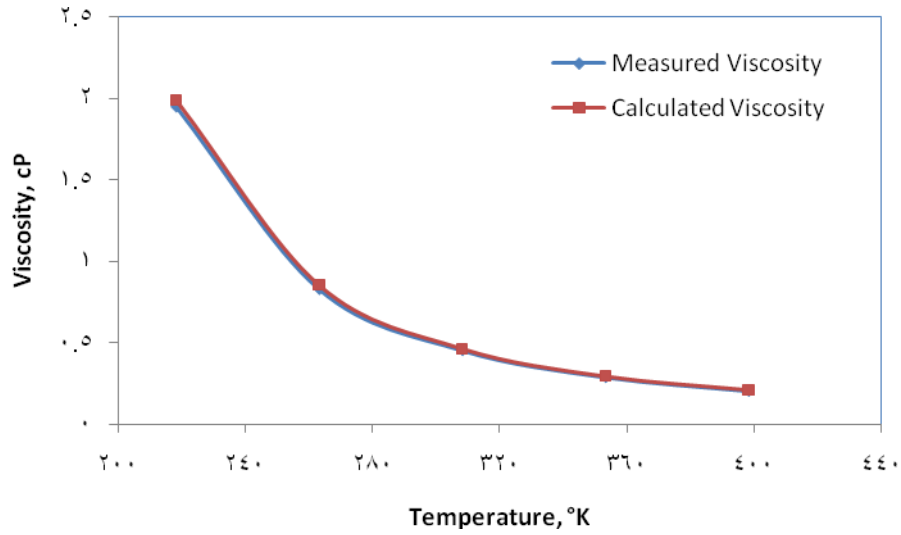
Figure 11: Comparison between measured and calculated viscosity for n-Octane.

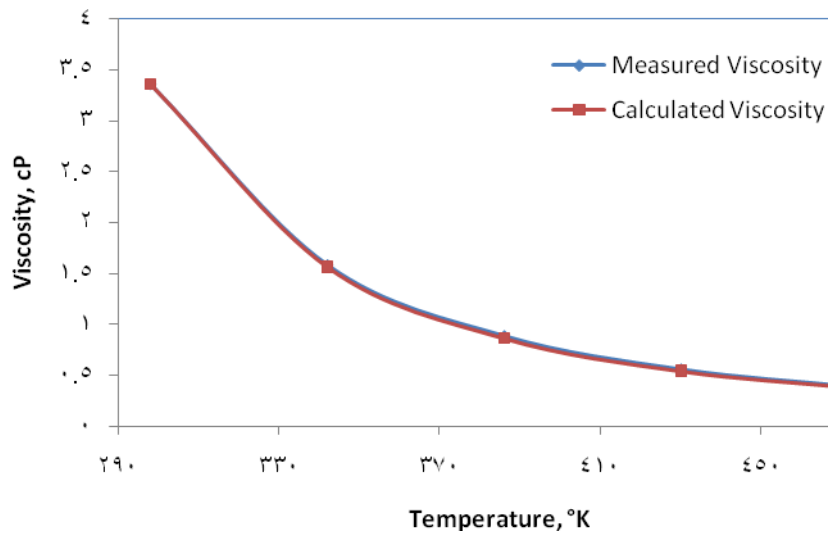*Figure 12: Comparison between measured and calculated viscosity for n-Nonane.*

Figure 13: Comparison between measured and calculated viscosity for n-Decane.

Figure 14: Comparison between measured and calculated viscosity for n-Undecane.
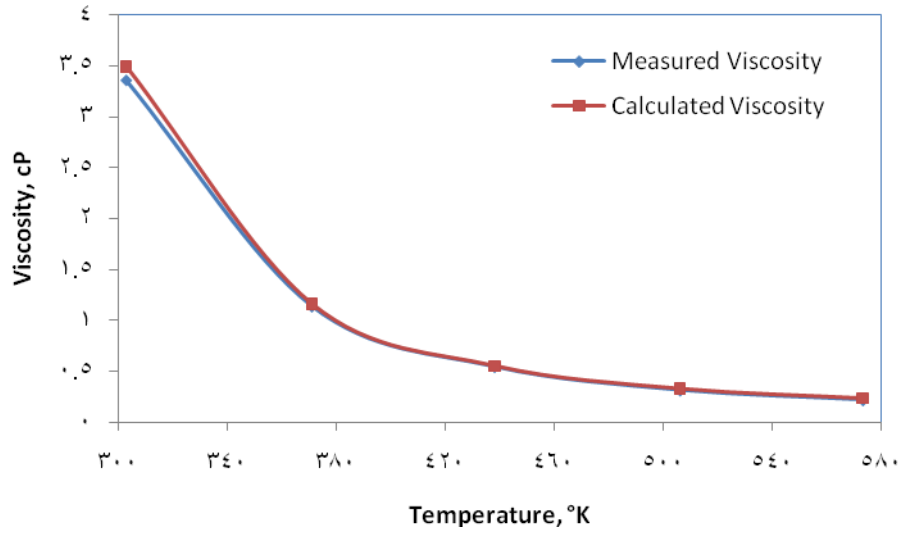
Figure 15: Comparison between measured and calculated viscosity for n-Dodecane.

Figure 16: Comparison between measured and calculated viscosity for n-Tridecane.

Figure 17: Comparison between measured and calculated viscosity for n-Tetradecane.

Figure 18: Comparison between measured and calculated viscosity for n-Pentadecane.

Figure 19: Comparison between measured and calculated viscosity for n-Hexadecane.

Figure 20: Comparison between measured and calculated viscosity for n-Heptadecane.

Figure 21: Comparison between measured and calculated viscosity for n-Octadecane.
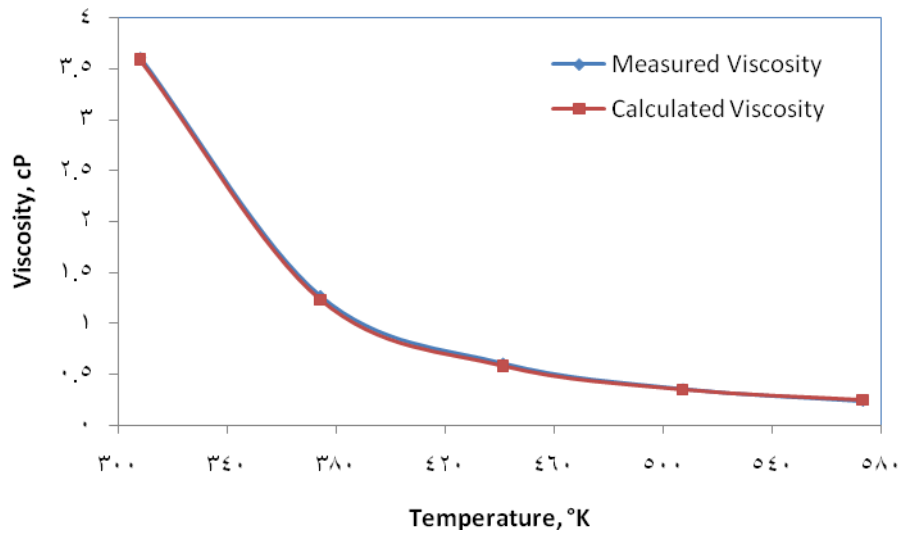

Figure 22: Comparison between measured and calculated viscosity for n-Nondecane.
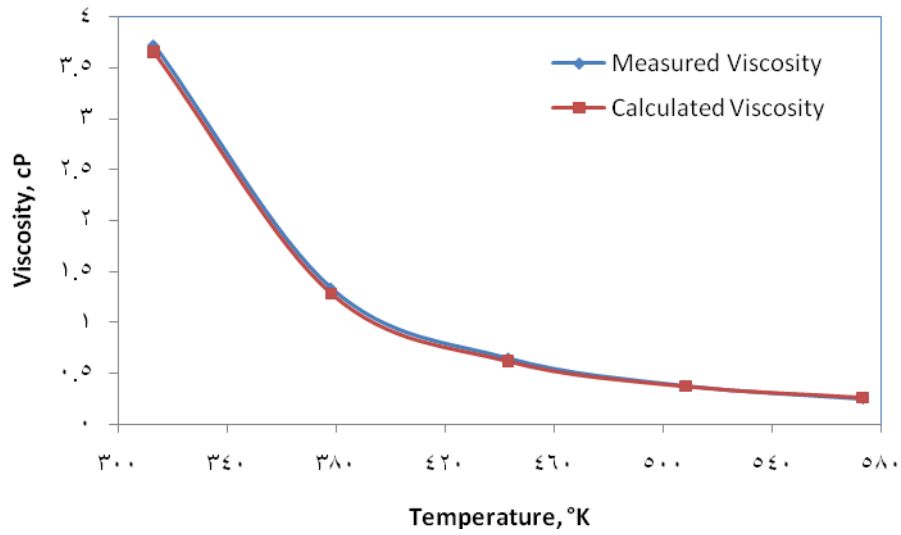
Figure 23: Comparison between measured and calculated viscosity for n-Eicosane.