IJCPE
Iraqi Journal of Chemical and Petroleum Engineering

Iraqi Journal of Chemical and Petroleum Engineering
Vol.12 No.4 (December 2011) 37-51
ISSN: 1997-4884

University of Baghdad

Improved Method to Correlate and Predict Isothermal VLE Data of Binary Mixtures

Venus Majeed Bakall Bashy Al-Temimi

Abstract

Accurate predictive tools for VLE calculation are always needed. A new method is introduced for VLE calculation which is very simple to apply with very good results compared with previously used methods. It does not need any physical property except each binary system need tow constants only. Also, this method can be applied to calculate VLE data for any binary system at any polarity or from any group family. But the system binary should not confirm an azeotrope. This new method is expanding in application to cover a range of temperature. This expansion does not need anything except the application of the new proposed form with the system of two constants. This method with its development is applied to 56 binary mixtures with 1120 equilibrium data point with very good accuracy. The developments of this method are applied on 13 binary systems at different temperatures which gives very good accuracy.

Keywords: *VLE, vapor liquid equilibrium, isothermal data prediction, new thermodynamic relation, VLE of binary mixtures.*

1. Introduction:

There are so many applications of VLE; therefore, techniques for calculation and experimental determination of this particular type of phase equilibrium are more highly developed than any other thermodynamic types. Therefore, this subject should be the first of the application to be mastered.

Besides the complexity of running VLE experiment at constant temperature it is expensive. Hence it would be of great advantage to be able to predict the shape of the VLE curve without the need to run an experiment. [1]

Many methods are suggested to predict VLE data which are summarized here.

2. Methods for VLE Calculation:

The methods usually used to calculate VLE data can be summarized as follows:

a. VLE Data from EOS:

EOS and CEOS have a theoretical aspect through the derivation. Many forms are introduced to calculate VLE data based on the required conditions, and the type of systems like RK EOS [2], SRK EOS [3], PR EOS [4], PRSV EOS [5], etc. Besides it is capable to represent vapor and liquid phases, it has many short comes. So, efforts are directed to improve it. VLE calculation by an EOS is difficult to treat unsymmetrical mixtures. Therefore, adjustable parameters are introduced in order to fit the experimental data. [6]

All the introduced adjustable parameter or parameters need an experimental data points in order to be evaluated at certain temperature and pressure. Another out-come appears through the calculation of VLE by EOS where for various systems there is a number of equations of states; each is specified to certain temperature and pressure ranges, polarity, or hydrocarbon cut. This is a reason why there are a very large number of equations of state instead of one EOS representing all systems in all conditions.

b. *Models to Predict VLE Data:*

These models are much more empirical in nature when compared to the property predicted from EOS which is typically used in the hydrocarbon mixtures. The tuning parameters of any activity models should be fitted against a representative sample of experimental data and their application which should be limited to moderate pressure and usually these constants are subjects to single temperature. Consequently, more caution should be exercised when selecting these models for particular simulation. The individual activity coefficient for any system can be obtained from derived expression for excess Gibbs Duhem equation. [7]

The early models (Margules [8], Van Laar [8]) provide an empirical representation of VLE and that limits their application. The newer models such as Wilson [9], NRTL [8], UNIQUAC [8], and UNIFAC [10] utilize the local composition concept and improvement in their general application and reliability. All these models involve the concept of binary interaction parameters and require that they be fitted to experimental data. [7]

The activity coefficient models are used as a tool for phase equilibrium calculations. All such models are empirical in nature and represent the activity coefficient of a component in a mixture (and hence its fugacity) in terms of an equation that contains a set of parameters. Two general approaches are employed:

i. The parameters of activity coefficient model are determined in a fit to experimental VLE data in a binary mixture; in this sense, these models are only a correlation for the binary systems. Although they may allow extrapolation with respect to temperature or pressure but it is truly predictive for multicomponent systems. Examples of these models are Wilson, TK-Wilson [8], NRTL, and UNIQUAC activity coefficient models.

ii. An alternative approach, which requires no experimental data, is one in which the parameters of the activity coefficient model are estimated by group contribution method. Several such schemes have been developed with functional group parameters determined by regression against a very large data base of experimental VLE results. Examples of these approaches are ASOG [11] and UNIFAC [10] models. [12]

3. New Method to Predict isothermal VLE Data:

Prediction of VLE data is one of the most important objects of researchers for centuries. Because of the difficulties associated with the experiments and the error might happen during the experiment. So, a predictive tool is needed.

This correlation is based on a statistical hypothesis and the flexibility of the proposed function to represent VLE data for a binary mixture at certain temperature.

Since all the previous method and approaches used to calculate or predict VLE data with numerical or physical base need constants in order to eliminate the deviation or error which appears in comprised with the experimental data. This method benefits from the mathematical behavior of exponential function when representing the VLE data of isothermal binary mixtures.

This method can calculate VLE data at any vapor composition at certain temperature with the need of two constants values for the binary at that temperature. The proposed function has the following form:

$$P = A\exp(B\,y) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where: P= saturation pressure for the selected binary mixture and is taken in mmHg for these constants.

A, and B= equation constants for specified mixture at certain temperature

y= vapor phase mole fraction

For any binary mixture, there are binary constant which are (A and B). These constants remain unchanged for the same binary mixture at certain temperature over the whole system composition; i.e, this simple relation can give P, x, y diagram representation for the binary mixture where x (liquid phase mole fraction) can be calculated by flash calculation. This method is very simple in application with reasonable accuracy if it is compared to previously used methods for VLE calculation. All of the used constants are specified for each system in order to match the experimental data in spite that some of them have a theoretical base. Besides the simplicity of the proposed equation, it can be applied to polar and non polar systems at any conditions and from any group except the mixtures which confirm azeotropes. Because of this limitation the proposed equation behaves as an exponential function. Also, the new form can be applied for all systems temperatures and compositions ranges. The proposed equation is applied on 56 different mixtures at different temperatures that range from different groups or families with 20 data points for each binary mixture at certain temperature; i.e, 1120 data points for all binary mixtures with very reasonable accuracy as shown in Table (1), where R^2 is called a recursion formula. It represents a statistical measure that represents the deviation from the proposed method. When R^2 approaches one, very good representation of equation is obtained. While, if recursion formula approaches zero, a very poor representation is obtained.

To see the graphical behavior of the proposed function which has a solid line representation with the experimental data representing figures by shapes for the whole system composition range at different temperatures. The figures are:

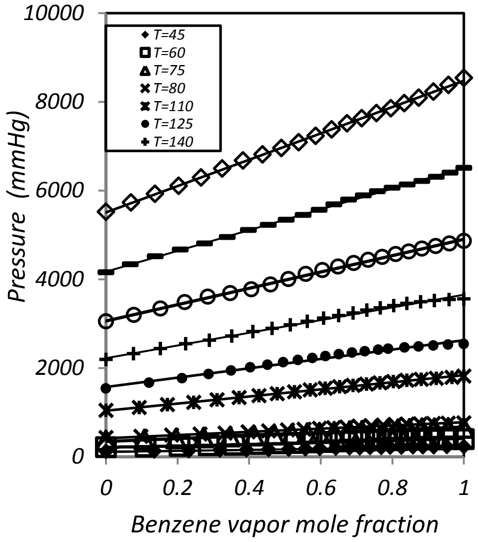


Fig. 1, n-Heptane + Benzene system

Table 1, new proposed equation constants and its accuracy

No.	***System*** [13]	***Temp. °C***	***Equation 1 constants***		***R^2***
			A	***B***	
1	*n-heptane + benzene*	45	115.7529	0.7278	0.9880
		60	213.6991	0.6677	0.9872
		75	363.5689	0.6311	0.9891
		80	436.0013	0.6071	0.9879
		110	1072.1799	0.5597	0.9893
		125	1609.5652	0.5102	0.9664
		140	2272.9713	0.4920	0.9848
		155	3123.5234	0.4659	0.9924
		170	4248.2850	0.4402	0.9947
		185	5607.0912	0.4258	0.9973
2	*n-heptane + Toluene*	25	30.3824	0.4636	0.9574
		30	38.9761	0.4530	0.9581
		40	62.1667	0.4434	0.9547
3	*n-heptane + 1-chlorobutane*	30	58.45	0.812	0.9970
		50	142.3911	0.7317	0.9965
		80	431.4	0.6419	0.9966
4	*n-butane + 1-butene*	37.8	2727.3818	0.1596	0.9179
		51.7	3860.5502	0.1777	0.9205
		65.6	5512.6930	0.1703	0.9344
5	*n-butane + 1,3-butadiene*	37.8	2727.3818	0.1596	0.9179
		51.7	3926.7768	0.1397	0.9205
		65.6	5600.6035	0.1341	0.9344
6	*n-octane + benzene*	55	42.0097	1.9801	0.9652
		65	83.3906	1.626	0.9669
		75	120.2414	1.6121	0.9715
7	*n-decane + toluene*	100.4	48.81	2.2036	0.9177
		110.5	75.7478	2.1146	0.9337
		120.6	127.9465	1.9380	0.9836
8	*carbon tetrachloride + toluene*	35	39.9962	1.3598	0.9671
		40	51.0098	1.3297	0.9691
		45	64.3979	1.2869	0.9707
		55	99.8127	1.2233	0.9730
		65	149.8724	1.1633	0.9756
9	*carbon tetrachloride + 2,4,4 trimethylpentane*	35	77.6443	0.8085	0.9964
		45	117.4508	0.7869	0.9937
		55	175.1214	0.7483	0.9914
		65	254.1325	0.7184	0.9905
10	*methanol + water*	35	35.7739	1.6956	0.9804
		39.8	45.0487	1.7007	0.9721
		50	78.8519	1.6149	0.9810
		60	131.2698	1.5336	0.9856
		65	173.1995	1.4649	0.9873
		100	728.2713	1.2615	0.9935
		140	2651.8723	1.1504	0.9974
11	*ethane + propane*	-145.5	0.0624	4.1169	0.7159
		-128.9	0.7112	3.5759	0.7752
		-101.1	11.836	2.9892	0.8839
		-73.3	96.7761	2.4878	0.8895
		-70	191.4197	2.0470	0.9678
12	*1,2dichloroethane + isoamylalcohol*	50	12.5169	2.7301	0.8899
		60	25.0624	2.4697	0.9134
		70	45.2774	2.2645	0.9288
		80	77.5508	2.0834	0.9422
13	*n-heptane + Ethylbenzene*	25	7.8495	1.6876	0.9759
		40	18.2654	1.5563	0.9796
		54.6	38.0839	1.445	0.9759

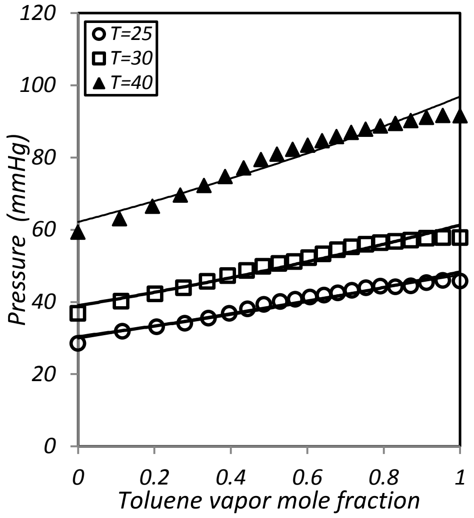


Fig. 2, n-Heptane + Toluene system

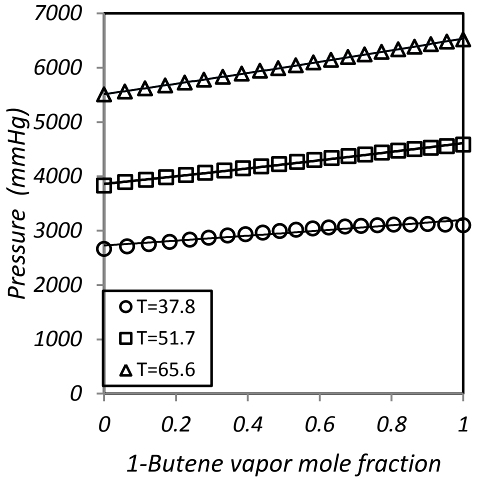


Fig. 5, n-Butane + 1-Butene system

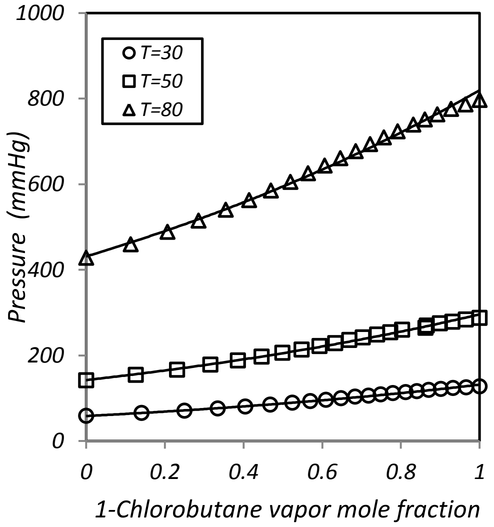


Fig. 3, n-Heptane + 1-chlorobutane system

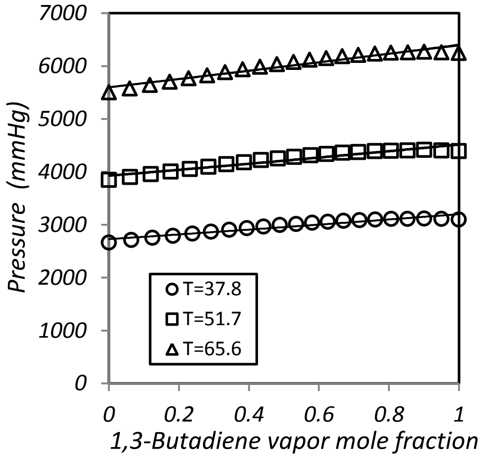


Fig. 6, n-Butane + 1,3-Butadiene system

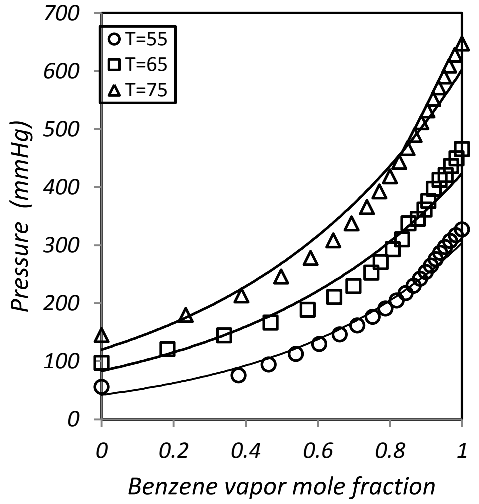


Fig. 7, n-Octane + Benzene system

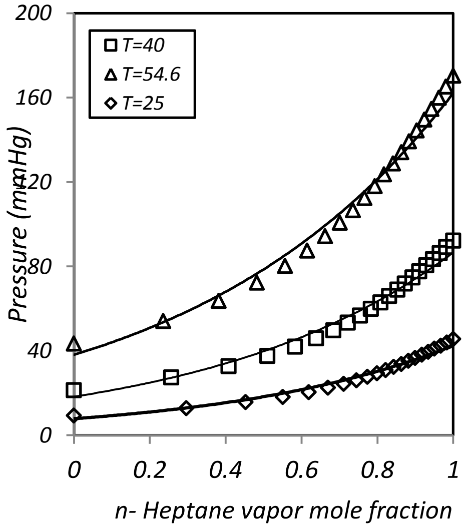


Fig. 4, n-Heptane + Ethylbenzene system

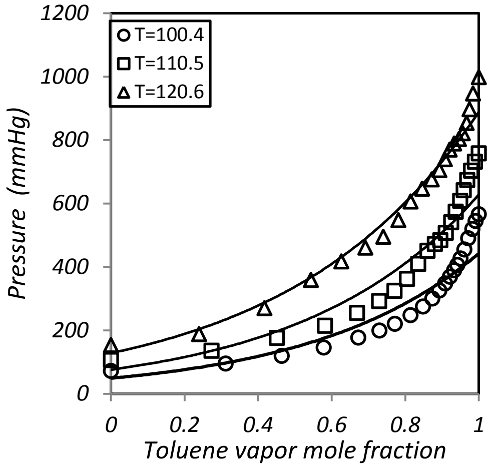


Fig. 8, n-Decane + Toluene system

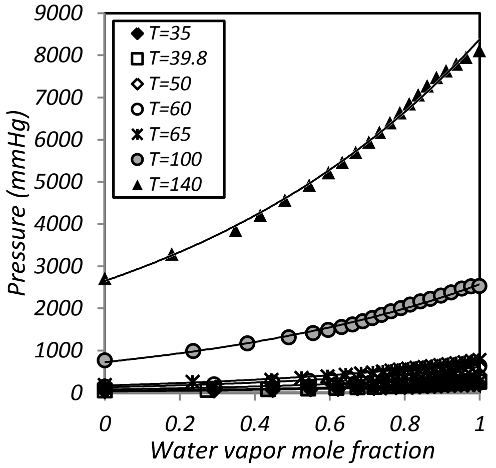


Fig.11, Methanol + Water system

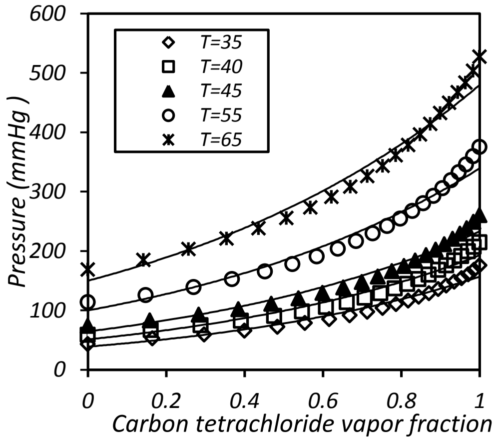


Fig. 9, Carbon tetrachloride + Toluene system

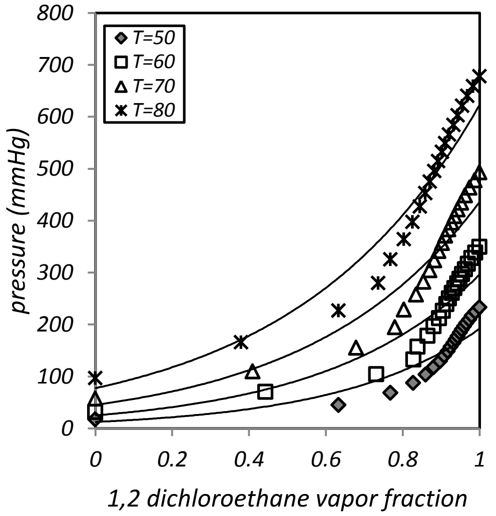


Fig. 12, 1,2 Dichloroethane + isoamylalcohole system

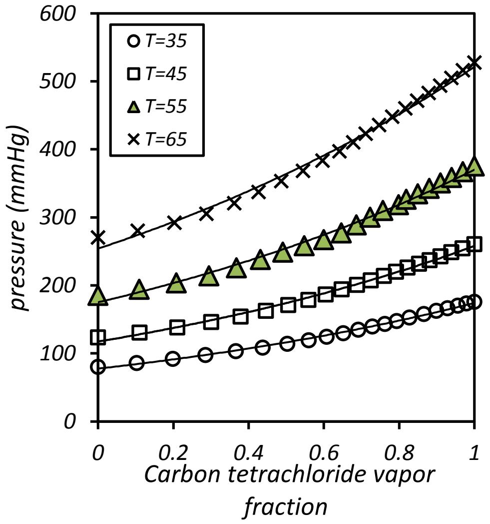


Fig. 10, Carbon tetrachloride +Trimethylpentane system

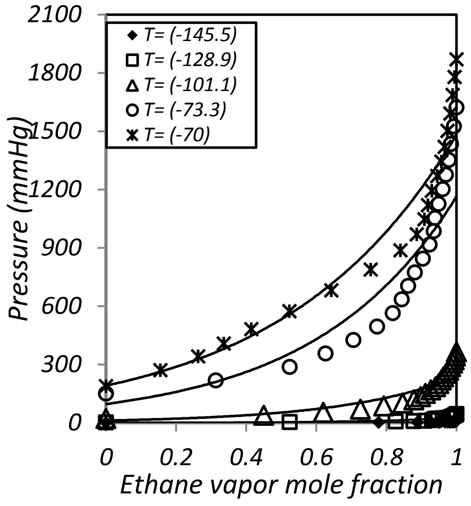


Fig.13, ethane + Propane system

4. Improving the New Proposed Function

In order to expand the applicability of the proposed equation, a new method is introduced. The improved method tries to calculate the equation constants at any temperature within a certain temperature range. It is noticed that *(A and B)* constants are functions of experiment temperature. The *A* and *B* proposed function or formulas have the following forms:

$$A = a\,e^{bT} \qquad \ldots\ldots\ldots\ldots(2)$$

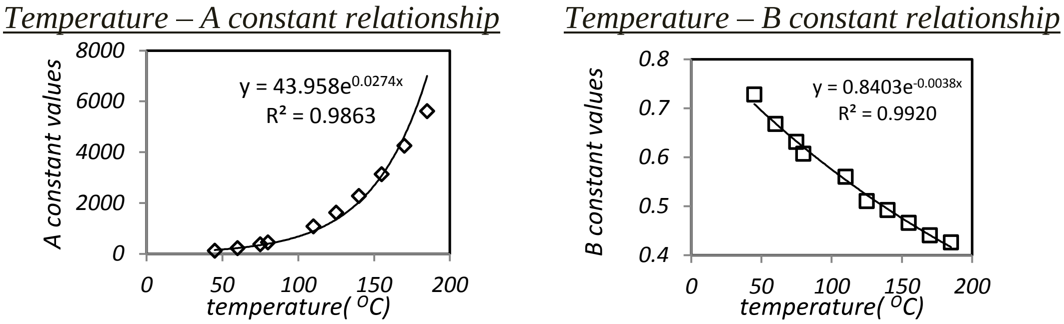
$$B = a^{*}\,e^{b^{*}T} \qquad \ldots\ldots\ldots\ldots(3)$$

Where: *A*, *B* : equation (1) constants values specified for each binary mixture

a, b, a^{*}, b^{*} : are new constants for each binary system at certain temperature range.

T : the required temperature measured in (°C) needed to calculate the constants.

The shape of the proposed relations and its fitting to the experimental data are given in the following figures:


Temperature – A constant relationship

Temperature – B constant relationship

Fig. 14, n-Heptane + Benzene system for A, and B constants relations

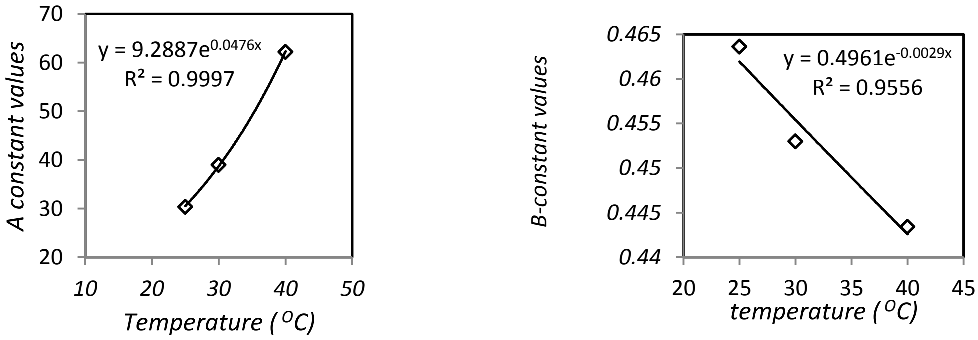


Fig. 15, n-Heptane + Toluene for A and B constants relations

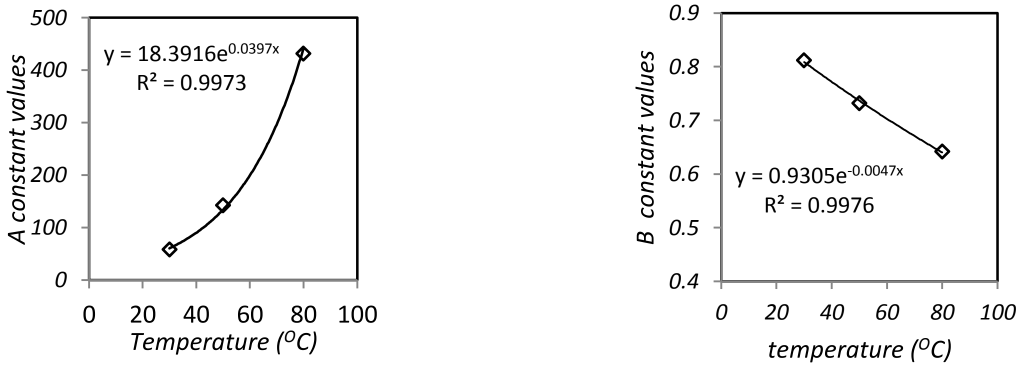


Fig. 16, n-Heptane + 1,Chlorobutane for A and B constants relations

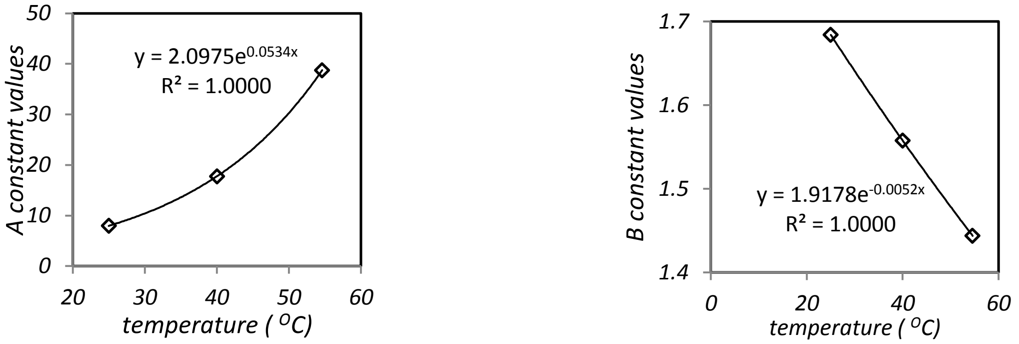


Fig. 17, n-Heptane + Ethylbenzene for A and B constants relations

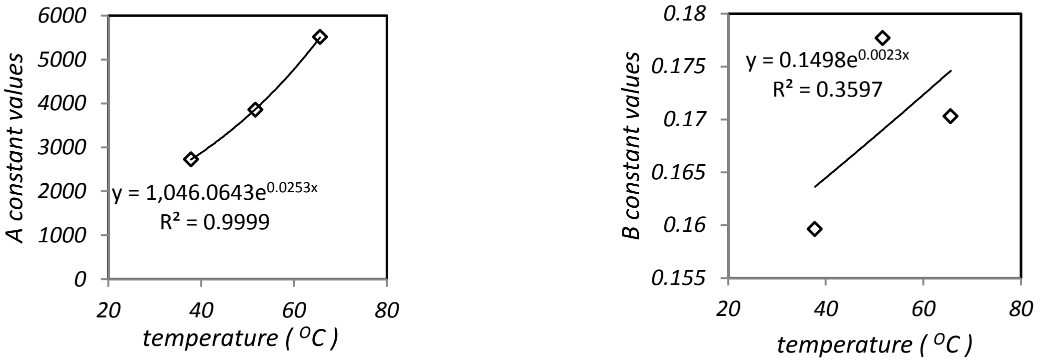


Fig. 18, n-Butane + 1-Butene for A and B constants relations

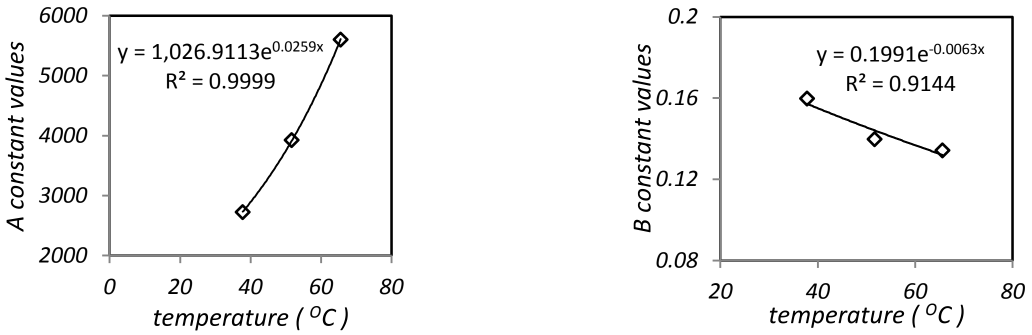


Fig. 19, n-Butane + 1,3-Butadiene for A and B constants relations

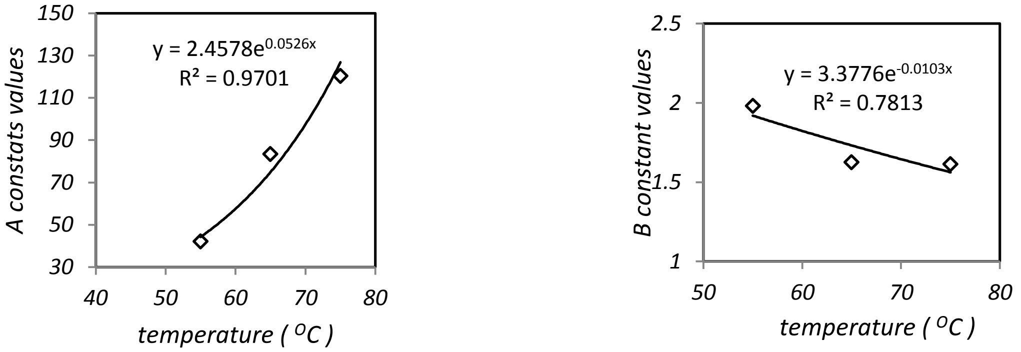


Fig. 20, n-Octane + Benzene for A and B constants relations

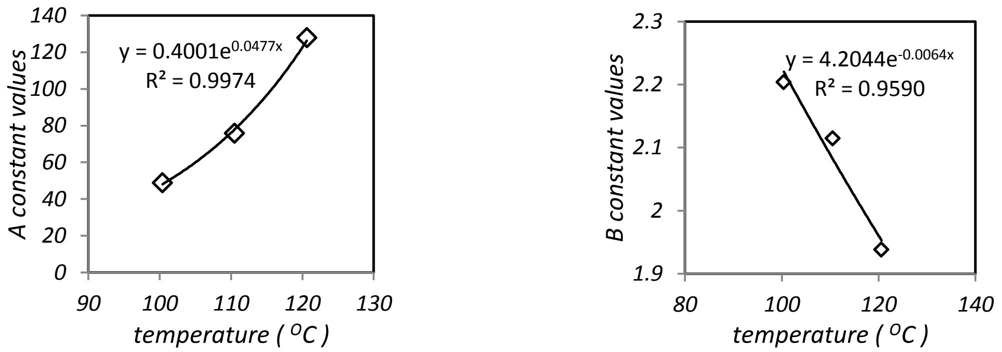


Fig. 21, n-Decane + Toluene for A and B constants relations

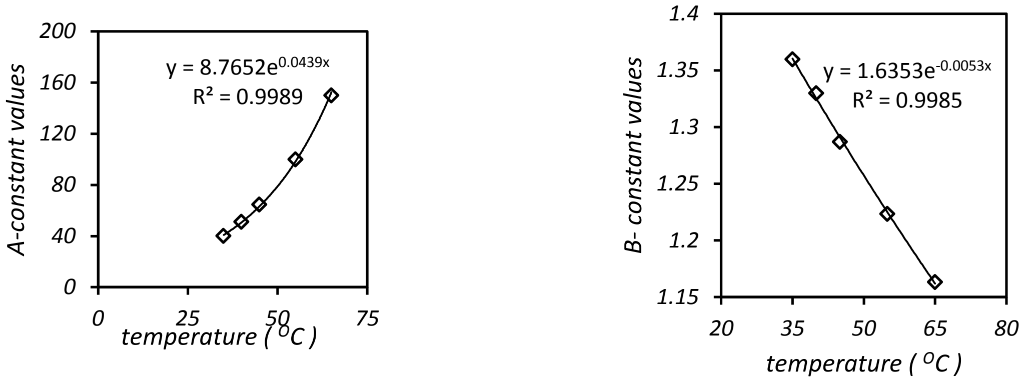


Fig. 22, Carbon tetrachloride + Toluene for A and B constants relations

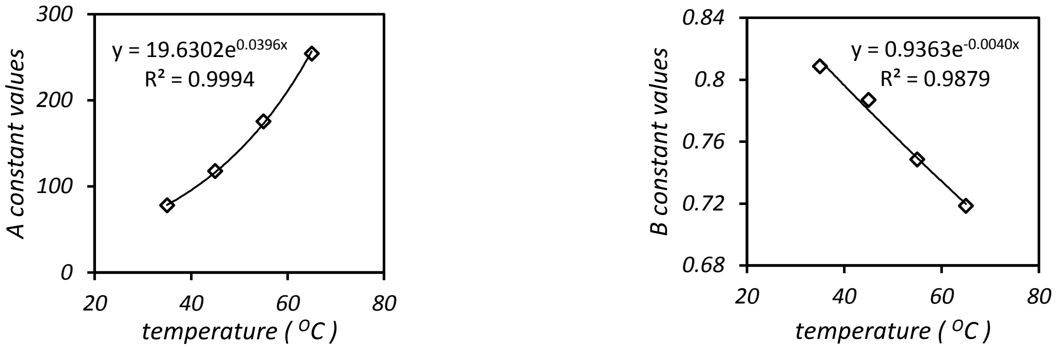


Fig. 23, Carbon tetrachloride + Trimethyl pentane for A and B constants relations

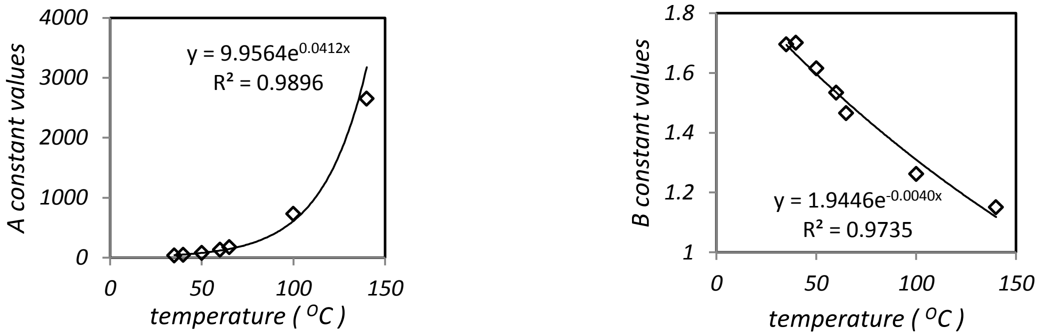


Fig. 24, Methanol + Water for A and B constants relations

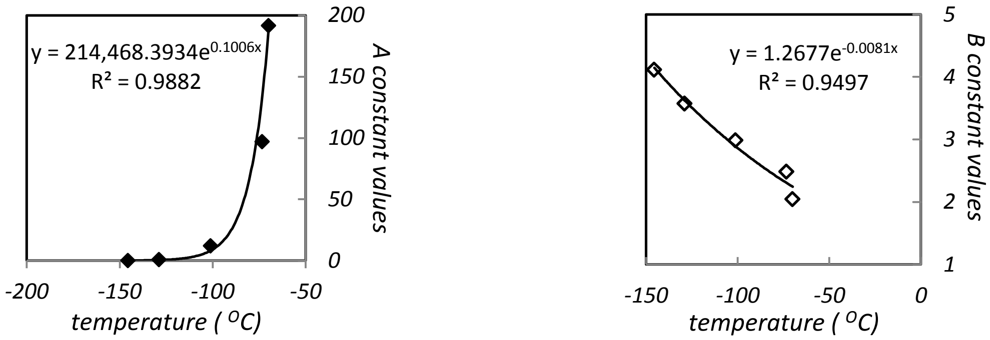


Fig. 25, Ethane + Propane for A and B constants relations

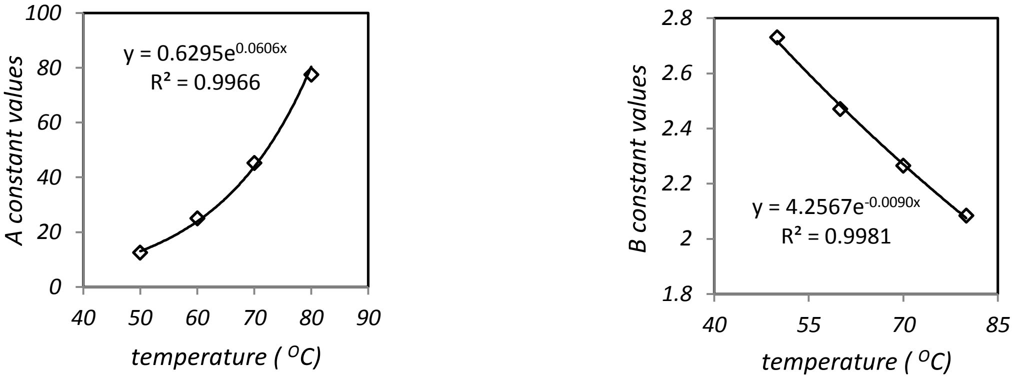


Fig. 26, 1,2-dichloro ethane + isomamyl alcohole for A and B constants relations

The improvement of the new method constants extend the application of system constant to a range of temperature depending on *a, b,* a^**, and* b^* as the calculated range for the heat capacity constants calculation. The new constants calculation method is applied on 13 systems with different temperatures range and from different groups or families as shown in Table (2).

Table (2) shows very good applicability for the extend temperature range. Now, if any researchers needs VLE data for a selected system at a selected temperature within the constant temperature range the following steps should be followed:

1. *Find constant a, b,* a^**, and* b^* *from a table* for a certain binary mixture.
2. *Select the required temperature which should be within the constant range.*
3. *Substitute the constants a, b and the temperature in eq 2 to calculate A constant.*
4. *Substitute the constants* a^**,* b^* *and the temperature in eq 3 to calculate B constant.*
5. *Substitute the obtained constants A and B in eq. 1 to calculate saturation pressure at any vapor mole fraction.*
6. *Make flash calculation at this temperature, pressure, and vapor mole fraction to calculate liquid mole fraction.*
7. *Draw P, x, and y figure and also, x, y figure.*

This method really lowers the experimental cost and the difficulty associated with the experiment where at high pressure the VLE experiment is very difficult to manage and expensive.

Table 2, The new improved relation constants

No.	system	No. of points	Temp. range °C	Eq. 2 constants A	Eq. 2 constants B	R^2	Eq. 3 constants a^*	Eq. 3 constants b^*	R^2
1	*n-heptane + benzene*	100	45_185	43.958	0.0274	0.9863	0.8403	-0.0038	0.992
2	*n-heptane + Toluene*	30	25_40	9.2887	0.0476	0.9997	0.4961	-0.0029	0.9556
3	*n-heptane + hlorobutane*	30	30_80	18.3916	0.0397	0.9973	0.9305	-0.0047	0.9976
4	*n-butane + 1-butene*	30	37.8_65.6	1046.0643	0.0253	0.9999	0.1498	0.0023	0.3597
5	*n-butane + 3-butadiene*	30	37.8_65.6	1026.9113	0.0259	0.9999	0.1991	-0.0063	0.9144
6	*n-octane + benzene*	30	55_75	2.4578	0.0526	0.9701	3.3776	-0.013	0.7813
7	*n-decane + toluene*	30	100.4_120.6	0.4001	0.0477	0.9974	4.2044	-0.0064	0.959
8	*carbon achloride + toluene*	50	35_65	8.7652	0.0439	0.9989	1.6353	-0.0053	0.9985
9	*carbon achloride + 2,4,4 ethylpentane*	40	35_65	19.6302	0.0395	0.9994	0.9363	-0.0040	0.9735
10	*methanol + water*	70	35_140	9.9564	0.0412	0.9896	1.9446	-0.0040	0.9735
11	*ethane + propane*	50	-145.5_-70	214468.3934	0.1006	0.9882	1.2677	-0.0081	0.9497
12	*1,2dichloro ethane + amylalcohol.*	40	50_80	0.6295	0.0606	0.9966	4.2567	-0.0090	0.9981
13	*n-heptane + thylbenzene*	30	25_54.6	2.0975	0.0534	0.9990	1.9178	-0.0052	0.9993

5. Discussion

Prediction of VLE data is one of the most important objectives of the researchers for centuries. Because of the difficulties associated with the experiments and because error might happen through the experiment, a predictive tool is needed.

Historically EOS is used to predict VLE data and the researchers tried to improve EOS in order to be capable of representing VLE data. Besides the capability of EOS to predict VLE data, it has many short comes. The most important of them is the incapability of EOS to represent all components and component mixtures; in other word the equations of state are classified according to component families or groups (polar, non-polar, ketones, hydrocarbons, heavy hydrocarbons, light hydrocarbons, alcohols …etc.) and also, according to the operation condition; i.e (system temperature and pressure).

Till the eighties of the past century, researchers turn to improve EOS approximately stopped and the improvement of EOS mixing rules was adopted. EOS mixing rules has also a short out-comes. Its short comes is that different forms depend on mixing rules. One of the most important short comes is that mixing rules share with it the adjustable parameter introduced in order to eliminate the deviation of each mixture from the ideal mixture which EOS hypothesis based on through its derivation. While, the other methods adopted to calculate VLE data have a number of constants specified for each system; this makes these methods also difficult to work with.

This work over comes all the short comings of EOS without any theoretical base but the need of two constants which represent the binary system mixture under the temperature range which the temperature constants accept it. So, the researchers can obtain very accurate experimental data points for any required temperature within the temperature range of the constants which represent that binary mixture. Besides its capability to represent VLE data with the system vapor pressure at any needed temperature this method is very simple to apply with very good accuracy compared with other used methods as will be seen in Table (3).

The improved relation is derived from the observation of the regular transmission behavior of the same mixture from temperature to another at constant pressure. This relation can be applied to all types of binary mixtures at any conditions except the mixtures which confirm azeotropes because the inabilities of the exponantional function to represent the VLE data of azeotropes. Also, from the table results one can observe that systems under very low temperatures or in other word negative experiment condition will give less accurate results compared with positive temperature of the experimental conditions results. Noting that these proposed relations is function to component with higher vapor pressure.

The error associated with the experimental data also affected the accuracy of the derived relation and this can be shown clearly when representing the data with poor R^2 factor for different binary mixtures.

This method compared with Antoine equation to calculate vapor pressure with the need to three constants. This method needs only these constants at certain temperature. Besides that, this method can be modified to calculate the vapor pressure of any binary mixture at any temperature with the need of four constants at acceptable range temperature. This improvement cannot be achieved by Antoine or any other equation with very good accuracy.

Table 3, Comparison between the accuracy of the systems after and before applying the improving of the proposed correlation

system	*Temp. (^{O} C)*	*A constant from eq. 2*	*B constant from eq. 3*	*ABE% at exact A, and B values eq.1*	*ABE% at general A, and B values eq. 2&3*
n-heptane + benzene	45	150.8426	0.7082	1.7707	2.8782
	60	227.5197	0.6690	1.6750	6.5731
	75	343.1736	0.6319	1.5005	5.5489
	80	393.5613	0.6200	1.5187	9.0305
	110	859.3699	0.5532	1.4256	1.6787
	125	1350.5091	0.5226	2.2304	1.5458
	140	2037.0071	0.4936	1.4271	1.0283
	155	3072.4695	0.4663	0.9856	1.7633
	170	4634.2836	0.4404	0.8001	9.1080
	185	699.0075	0.4160	0.5687	2.3999
Over all ABE%				*1.39024*	*4.15547*
n-heptane + Toluene	25	30.53271	0.4614	2.2558	2.2695
	30	38.73713	0.4548	2.1803	2.2935
	40	62.35218	0.4418	2.2927	2.2831
Over all ABE%				*2.2429*	*2.2820*
n-heptane + 1-chlorobutane	30	60.5152	0.8081	0.8944	3.1636
	50	133.8733	0.7356	1.0102	6.1097
	80	440.4928	0.6389	0.8709	1.8830
Over all ABE%				*0.92517*	*3.7188*
n-butane + 1-butene	37.8	2721.854	0.1634	1.1944	1.1945
	51.7	3868.951	0.1687	0.2633	0.4284
	65.6	5499.479	0.1742	0.0779	0.0977
Over all ABE%				*0.51187*	*0.57353*
n-butane + 1,3-butadiene	37.8	2733.48	0.1569	1.1944	1.2178
	51.7	3918.017	0.1437	1.0293	1.0251
	65.6	5615.865	0.1317	0.8956	0.8785
Over all ABE%				*0.70643*	*1.04047*
n-octane + benzene	55	49.5091	1.6523	6.2710	11.8731
	65	78.3477	1.4509	6.9992	6.9904
	75	123.9846	1.2740	6.0223	9.0550
Over all ABE%				*6.43083*	*9.30617*
n-Decane + toluene	100.4	48.0883	2.2113	14.3077	13.4844
	110.5	77.85197	2.0729	11.9136	11.8038
	120.6	126.0375	1.9431	4.8759	4.5214
Over all ABE%				*10.36573*	*9.93653*
carbon tetrachloride + toluene	35	40.7432	1.3584	5.5607	5.0466
	40	50.7438	1.3229	5.6526	5.2520
	45	63.1991	1.2883	5.2505	5.1291
	55	98.0316	1.2218	4.8305	5.2396
	65	152.0622	1.1587	4.4040	6.4604
Over all ABE%				*5.13966*	*5.42554*
carbon tetrachloride + 2,4,4 trimethylpentane	35	78.4977	0.8085	1.2127	1.5779
	45	116.6373	0.7821	1.3823	1.4740
	55	173.3078	0.7514	1.6183	1.7135
	65	257.5127	0.7219	1.5679	2.4187
Over all ABE%				*1.4453*	*1.79603*
methanol + water	35	42.1071	1.6906	4.6667	6.8630
	39.8	51.3146	1.6584	5.7752	4.6207
	50	78.8519	1.5921	4.3085	4.7792
	60	117.9447	1.5297	3.6429	5.3192

	65	144.9249	1.4994	3.3458	7.1379
	100	612.9084	1.3035	2.2133	6.5336
	140	3185.025	1.1108	1.2889	8.9827
Over all ABE%				*3.6059*	*6.3195*
ethane + propane	-145.5	0.0943	4.1196	23.0094	17.3828
	-128.9	0.5009	3.6013	17.4166	31.7519
	-101.1	8.20922	2.8752	13.6966	33.4154
	-73.3	134.5502	2.2955	9.15259	10.4304
	-70	187.526	2.2349	6.4944	6.7880
Over all ABE%				*13.9539*	*19.9537*
1,2dichloroethane + isoamylalcohol	50	13.0289	2.7142	6.2004	7.3514
	60	23.8831	2.4806	3.4433	4.6633
	70	43.7797	2.2671	6.2076	2.1002
	80	80.2519	2.0720	5.2163	9.5582
Over all ABE%				*5.2669*	*5.9183*
n-Heptane + Ethylbenzene	25	7.9705	1.6840	5.2406	3.9192
	40	17.7564	1.5577	4.5968	5.1011
	54.6	38.7212	1.4438	3.8001	3.9025
Over all ABE%				*4.54583*	*4.3076*
All systems over all ABE%				***4.3485***	***5.7487***

6. Conclusion

- The proposed relation can represent VLE data without a need to any other relation except two constants that represent each binary system at the specified temperature like any other constants introduced through historically used relations.
- The improving of this relation made it very elastic in representing a very large rang of VLE data of the binary systems.
- The derivation of the constants should cover the required calculated VLE temperature.
- When the temperature range increases the error slightly increases.
- The results of calculation show that constant A has a more effect than B on the accuracy of calculated VLE data.
- The obtained error might be from the experimental error causing an error through VLE calculation.
- The calculated constants are functions of the component and experimental temperature.
- This equation can calculate the systems with higher vapor pressure without the need to run an experiment.
- Experiment run under negative temperature will give less accurate results compared with that at positive experimental temperature.

Abbreviations

ABE	Average absolute error
CEOS	Cubic equation of state
EOS	Equation of state
VLE	Vapor liquid equilibrium

References:

1. Harold A. Beaty, and George Calingaert, (1934), "Vapor Liquid Equilibrium of Hydrocarbon Mixtures", Ind. And Eng. Chem., vol. 26, No. 5, PP. (504)
2. Smith, J. M., Van Ness, H.C., Abbott, M. M., (2004), "Introduction to chemical engineering thermodynamics", McGraw-Hill companies.
3. Soave, G., (1972), "Equilibrium constants from a modified RK EOS", chem. Eng. scie., vol. (27), PP. (1197).
4. Ding-yu Peng, and Donald B. Robinson, (1976), " A New two

constants EOS", Ind. Eng. Fandam., vol. 15, no. 1, PP. (59).

5. Stryjek, R., and Vera, J. H., (1986), "PRSV: An Improved PR EOS of pure components and mixtures", the cand. J. of chem. Eng., vol.64, PP. (323).
6. Soave, G., (1993), "20 years of RK EOS", fluid phase equilibrium, vol. 82, PP. (345).
7. Hysys company, (2001), "property Methods and calculation"), ver. 2 manual
8. Smith, J. M., Van Ness, H.C., Abbott, M. M., (1996), "Introduction to chemical engineering thermodynamics", McGraw-Hill companies.
9. Wilson, G. M., (1964), J. Am. Chem. Soc., vol. 86, PP. (127).
10. Gmehling, J., and Rasmussen, P., and Fredenslund, Aa, (1982), "VLE by UNIFAQ group contribution revision and extension 2", IEC. Process Des. Dev., vol. 21, PP. (118).
11. Soave, G., (1993), "Application of EOS and the theory of group solutions to phase equilibrium prediction", fluid phase equilibrium, vol.47, PP. (189).
12. Marc, J. Assael. Martin Trusler, J. P.: Thomas F. Tsolakis, (1996), "thermophysical properties of fluids", published by ICP, London.
13. Shuzo ohe, (1989), "VLE Data", physical data science 37, published by Elsevier, Tokyo, Japan.

تطوير طريقة جديدة لربط و استحصال نقاط توازن البخار مع السائل عند درجة حرارة ثابتة للخلائط الثنائية

من قبل د. فينوس مجيد بقال باشي التميمي

ايجاد طريقة لحساب توازن البخار و السائل دائما تحتاج. قدمت طريقة جديدة لحساب توازن البخار مع السائل وكانت باسلوب سهل جدا" وأعطت نتائج جيدة جدا" مقارنة مع الطرق التي أستخدمت سابقا" بدون الحاجة الى اي خاصية فيزياوية لأي من المركبات . ما عدا الحاجة الى ثابتان اثنان فقط يمثلان ذلك الخليط. بالأضافة الى انه هذه الطريقة ممكن تطبيقها لحساب توازن البخار مع السائل لأي خليط ثنائي بأي قطبية و من أي مجموعة على عكس الطرق السابقة. ما عدا الخلائط التي تكون مركبات ايزوتروبية. هذه الطريقة قد طورت لتشمل شكل جديد بحيث تغطي مدى من درجات الحرارة. هذا المدى لايحتاج خلال التطبيق سوى ثابتين فقط. وقد تم تطبيق المعادلة المقترحة على 56 مركب عند درجات حرارة مختلفة لـ 1120 نقطة توازن مختبرية وكانت النتائج جيدةجدا". بينما تطوير الطريقة طبق على 13 مزيج ثنائي عند درجات حرارة مختلفة واعطت نتائج جيدة جدا".