GROUP CONTRIBUTION METHOD FOR THE ESTIMATION OF CRITICAL PROPERTIES OF SOME LINEAR ALIPHATIC DIMETHYL ESTERS OF DICARBOXYLIC ACIDS

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Abstract: Critical temperature (T_c), critical pressure (P_c) and critical volume (V_c) of the linear aliphatic dimethyl esters of dicarboxylic acids $CH_3-CO_2-(CH_2)n-CO_2-CH_3$ (with n = 0 to 8) were estimated using Group Contribution Methods. Experimental data on the critical properties were compared with the estimations by group contributory methods of Lydersen, Constantinou and Gani, and Marrero and Gani. In the case of T_c, predictions by the three methods showed average relative deviations (ARD) of 12.16, 19.85 and 13.35%, respectively. P_c estimations by the methods recorded deviations (ARD) of 2.72, 13.37 and 2.14%, respectively. Experimental data for V_c were not available for comparison. The need to expand the databank of critical properties of organic compounds that are vital in the design of process plants, underscores the essence of this study.

Keywords: Critical properties, dicarboxylic acids, dimethyl esters, group contribution

Introduction

Critical constants like critical temperature (T_c), critical pressure (P_c) and critical volume (V_c) are pivotal in the prediction of many transport and thermodynamic properties of compounds. For instance, the vapour pressure of most organic compounds can be extrapolated to the critical point if the T_c and P_c of the compounds are known (Verevkin *et al*., 2006). Reliable experimental data for some of the thermodynamic or pure component properties of many organic compounds are not so easy to come by. It is sometimes not feasible to determine them experimentally because many organic compounds are thermally labile, decomposing at temperatures near or below their critical temperatures. Critical temperatures higher than about 750/K cannot be determined accurately (Fisher, 1989). Several Group Contribution (GC) schemes have been advanced in cases where it is impossible to determine properties of substances experimentally. The critical properties of dimethyl esters of dicarboxylic acids are difficult to measure experimentally. Kudchadker *et al.* (2001), measured critical properties only for dimethyl oxalate. There is very little detail about the thermal stability of dimethyl esters of dicarboxylic acids in the open literature (Verevkin *et al*., 2006). Estimation of thermodynamic properties and prediction of properties at the critical boundary of compounds should not be performed perfunctorily. When a method for property prediction is faulty or inaccurate, a conspicuous variation between prediction and experiment becomes inevitable. The process engineer is often required to select from the best set of critical or thermodynamic property data for a vast array of mixtures and pure compounds (Constantinou & Gani, 1994). The objective of this work is the prediction of critical properties of the linear aliphatic dimethyl esters of dicarboxylic acids, by means of predictive methods based on group contribution. Three GC methods were tested for critical property prediction, namely; the methods of Lydersen (1955), Constantinou and Gani (1994) and Marrero and Gani (2001).

Theoretical Framework

Group Contributory methods are widely employed in the estimation of physical and thermodynamic properties of compounds. The compound is fragmented into structural groups (e.g. CH_3, CH_2, OH etc.). The contributions of the structural groups are summed up to obtain the property in question. Predictive capability of a method requiring contributions from groups of atoms appreciates with availability of necessary details about the molecular

configuration of a compound (Moller, 2007). Basic features of the molecular configuration of compounds are known to be identical in many different molecules; this is the footing for developing GC methods (Constantinou & Gani, 1994). Properties of thousands or millions of components are estimated from data for a few dozens or few hundreds of groups of atoms (Constantinou & Gani, 1994; Cedeño *et al.,* 2000; Marrero & Gani, 2001; Gani *et al.,* 2005; Monago & Otobrise, 2010; Cunico *et al.,* 2013).

As examples of the use of these methods, Bogdanic (2006) had predicted density, solubility, melting temperature and glass transition temperature of polymer systems using several GC methods. Sales-Cruz *et al.* (2010) used GC methods of Joback and Reid (1983), Constantinou and Gani (1994), Marrero and Gani (2001) the modified Rackett method (Spencer and Danner, 1972) and the GC method of Ceriani *et al.* (2007) to predict critical properties, density and viscosity of some fatty acids, triacylglycerols and methyl esters. Barley and McFiggans (2010), employed GC methods to estimate boiling temperatures for a set of compounds relevant to the formation of atmospheric aerosol. Acree and Chickos (2006) developed a GC method for the prediction of vapour pressures of solid organic compounds. Their method for total solid-to-liquid phase change entropy gave much better entropy predictions for the database examined, than the method earlier developed by Coutsikos *et al.* (2003). Lemmon and Goodwin (2000) reported a correlation for estimating the vapour pressures of n-alkanes from methane through n-hexatriacontane and isomers of butane to nonane. Owczarek and Blazej (2006) employed six GC methods to calculate the critical pressures of 180 saturated and unsaturated aliphatic hydrocarbons. The study also presented 95 recommended experimental data for the set of hydrocarbons. Ruzicka and Domalski (1993) estimated the heat capacities of organic liquids as a function of temperature using group additivity.

Recently, Montagud *et al.* (2017) presented two models based on a group contribution method, using a classical approach and neural networks, to predict the critical temperature, critical pressure, normal boiling temperature, acentric factor, and ideal gas heat capacity of organic fluids containing chlorine and/or fluorine. For all the properties studied the models showed a mean reduction of the absolute relative deviation (ARD) of more than 50%, in comparison with other methods. Petters *et al.* (2016) predicted the cloud condensation nuclei activity for organic compounds using functional group contribution methods. The study revealed that, hydroxyl, carboxyl, aldehyde, hydroperoxide, carbonyl,

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and ether moieties promote cloud condensation nuclei activity while methylene and nitrate moieties inhibit cloud condensation nuclei activity. Lazzús (2016) developed a simple GC method for the prediction of the freezing point of a number of ionic liquids. The results showed an average deviation of 5% when compared with experimental data that were available in the literature. Taherifard and Raeissi (2016) developed an easy and universal atomic GC method for the estimation of liquid densities of ionic liquids as a function of temperature and pressure. The method achieved an average absolute relative deviation of 0.95% from available experimental data. Albert and Muller (2014) evolved an estimation scheme for the heat capacity and thermal conductivity of ionic liquids. A mean absolute error of 5.4% was recorded in the case of heat capacity, for the reproducible data of the ionic liquids from the subset not used for the fitting. In the same vein, a mean absolute error of 8.1% was recorded by the authors for thermal conductivity of the ionic liquids.

Numerical Methods
Lydersen's estimation method employs structural contributions to estimate T_c, P_c and V_c. The relations are as follows:

$$T_c = T_b \left[0.567 + \Sigma \Delta_T - \left(\Sigma \Delta_T \right)^2 \right]^{-1} \quad [1]$$

$$P_c = M \left(0.34 + \Sigma \Delta_p \right)^{-2} \quad [2]$$

$$V_c = 40 + \Sigma \Delta_v \quad [3]$$

The units employed are Kelvin, atmosphere and cubic centimeter per mole for T_c, P_c and V_c respectively. The Δ quantities are evaluated by summing contributions for various atoms or groups of atoms. A table of Lydersen's critical property increments for various atoms or groups can be readily sourced (Reid *et al.*, 1977). To employ Lydersen's method, only the normal boiling point and the molar mass (M) are needed. Errors associated with these relations vary.

The estimation method of Constantinou and Gani uses second-order, as well as first-order groups to portray the minute differences in molecular structure of compounds and variations between isomers. The method has the added advantage of not requiring the normal boiling point for the prediction of critical temperature. "Let C_i be the contribution of the first – order group type – i, which occurs N_i times and D_j be the contribution of the second – order group type – j, which occurs M_j times in a compound. With $f(x)$ a simple function of the property *X*, the property estimation model takes the form of Eqn. 4

$$f(x) = \sum_i N_i C_i + W \sum_j M_j D_j \quad [4]$$

The constant *W* is assigned the value of unity in the second – order approximation, where both first and second – order group contributions are involved, and zero (0) in the first – order approximation, where only the contributions of the first – order groups are employed" (Constantinou and Gani, 1994). The function f(*x*) in Eqn. (4) for T_c is given by f(*x*) = *exp* (T_c/t_{co}). Hence, Eqn. (4) can be written as;

$$\exp(T_c / t_{co}) = \sum_i N_i C_i + W \sum_j M_j D_j \quad [5]$$

$$\therefore T_c = t_{co} \ln \left[\sum_j N_i C_i + W \sum_j M_j D_j \right] \quad [6]$$

t_{co} is a universal constant (adjustable parameter) with the value 181.128 K.

The function f(*x*) in Eqn. (4) for P_c is given by f(*x*) = $(P_c - P_{c1})^{-0.5} - P_{c2}$. Hence, Eqn. (4) can be written as:

$$\left(P_c - P_{c1} \right)^{-0.5} - P_{c2} = \sum_j N_i C_i + W \sum_j M_j D_j \quad [7]$$

$$P_c = P_{c_1} + \cfrac{1}{\left(P_{c_2} + \Sigma_i N_i C_i + W \sum_j M_j D_j \right)^2} \quad [8]$$

P_{c1} and P_{c2} are universal constants (adjustable parameters) with values 1.3705 bar and 0.100220 bar$^{-0.5}$ respectively.
The function f(*x*) in Eqn. (4) for V_c is given by f(*x*) = $V_c - V_{co}$. Hence, Eqn. (4) can be written as

$$V_c - V_{co} = \sum_i N_i C_i + W \sum_j M_j D_j \quad [9]$$

V_{co} is a universal constant (adjustable parameter) with a value of -0.004350 m^3/Kmol.
A table of the contributions for various atoms or groups as proposed by Constantinou and Gani can be readily sourced (Constantinou and Gani, 1994).

Marrero and Gani's estimation method was developed for the prediction of properties of pure organic compounds. Prediction is done at three levels. At the first level, contributions from simple groups, which enable the description of a number of organic compounds, are used. The second and third levels involve polyfunctional and structural groups, which give more details about different molecules and isomers. "The property-estimation model has the form of Eqn. 10

$$f(x) = \sum_i N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \quad [10]$$

In Eqn. (10), C_i is the contribution of the first-order group of type-i that occurs N_i times, D_j the contribution of the second-order group of type-j that occurs M_j times and E_k the contribution of the third-order group of type-k that has O_k occurrences in a compound. In the first level of estimation, the constants w and z are assigned zero values because only first-order groups are employed. In the second level, the constants w and z are assigned unity and zero values, respectively because only first- and second-order groups are involved while in the third level, both w and z are set to unity values" (Marrero and Gani, 2001).
The function f(*x*) in Eqn. (10) for T_c is given by f(*x*) = *exp* (T_c/t_{co}). Hence, Eqn. (10) can be written as;

$$\exp(T_c / t_{co}) = \sum_i N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \quad [11]$$

$$\therefore T_c = t_{co} \ln \left[\sum_j N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \right] \quad [12]$$

t_{co} is a universal constant (adjustable parameter) with the value 231.239 K.
The function f(*x*) in Eqn. (10) for P_c is given by f(*x*) = $(P_c - P_{c1})^{-0.5} - P_{c2}$. Hence, Eqn. (10) can be written as:

$$\left(P_c - P_{c1} \right)^{-0.5} - P_{c2} = \sum_j N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \quad [13]$$

$$P_c = P_{c_1} + \cfrac{1}{\left(P_{c_2} + \Sigma_i N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \right)^2}$$
$$[14]$$

P_{c1} and P_{c2} are universal constants (adjustable parameters) with values 5.9827 bar and 0.108998 bar$^{-0.5}$, respectively.

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The function f(x) in Eqn. (10) for V_c is given by f(x) = V_c - V_{co}. Hence, Eqn. (10) can be written as;

$$V_c - V_{co} = \sum_i N_i C_i + W \sum_j M_j D_j + Z \sum_k O_k E_k \quad [15]$$

V_{co} is a universal constant (adjustable parameter) with a value of 7.95 cm³/mol.

A table of the contributions for various atoms or groups as proposed by Marrero and Gani can be readily sourced (Marrero and Gani, 2001).

The deviation of estimated properties from experimental data for each dimethyl ester was calculated using the relation in Eqn. 16

$$D = \frac{Experimental_{(data)} - Calculated_{(data)}}{Experimental_{(data)}} \times 100 \quad [16]$$

Results and Discussions

Tables 1 – 3 contain the thermophysical properties predicted by the three GC methods. The general trend for most estimation methods is that, for organic compounds, as the number of carbon atoms (N_c) increases, T_c and V_c increases, while P_c decreases. In this work, the T_c calculated by Lydersen's method did not follow this trend, but the trend was observed for P_c. The results for T_c and P_c estimations by the methods of Constantinou and Gani as well as Marrero and Gani, were in agreement with the common trend.

Table 1: Properties predicted by the method of Lydersen

Dimethyl Ester	Nc	T_c/K	P_c/bar	V_c/m³mol⁻¹
dimethyl oxalate	4	638.31910	39.76490	0.00031
dimethyl malonate	5	651.09770	34.78050	0.00037
dimethyl succinate	6	665.51850	30.90120	0.00042
dimethyl glutarate	7	519.79360	27.79730	0.00048
dimethyl adipate	8	520.94380	25.25810	0.00053
dimethyl pimelate	9	529.31750	23.14270	0.00059
dimethyl suberate	10	715.15060	21.35340	0.00064
dimethyl azelate	11	560.10780	19.82030	0.00070
dimethyl sebacate	12	556.44210	18.49220	0.00075

Table 2: Properties predicted by the method of Constantinou and Gani

Dimethyl Ester	Nc	T_c/K	P_c/bar	V_c/m³mol⁻¹
dimethyl oxalate	4	489.07000	43.79900	0.31749
dimethyl malonate	5	506.65000	39.32800	0.37325
dimethyl succinate	6	522.36000	35.60600	0.42901
dimethyl glutarate	7	536.55000	32.47400	0.48477
dimethyl adipate	8	549.50000	29.81300	0.54053
dimethyl pimelate	9	561.40000	27.53500	0.59629
dimethyl suberate	10	572.41000	25.56800	0.65205
dimethyl azelate	11	582.66000	23.85800	0.70781
dimethyl sebacate	12	592.24000	22.36300	0.76357

Table 3: Properties predicted by the method of Marrero and Gani

Dimethyl Ester	Nc	T_c/K	P_c/bar	V_c/m³mol⁻¹
dimethyl oxalate	4	523.70500	39.62700	0.00031
dimethyl malonate	5	543.69200	34.90400	0.00036
dimethyl succinate	6	561.89800	31.10900	0.00042
dimethyl glutarate	7	578.61400	28.01500	0.00048
dimethyl adipate	8	594.06500	25.46000	0.00053
dimethyl pimelate	9	608.42900	23.32400	0.00059
dimethyl suberate	10	621.85000	21.52100	0.00064
dimethyl azelate	11	634.44400	19.98600	0.00070
dimethyl sebacate	12	646.30600	18.66700	0.00076

As stated in the introductory section, experimental data on the critical properties of the dimethyl esters are not readily sourced. Information about their thermal stability is scanty. However, Verevkin *et al*. (2006), determined the critical temperatures and pressures of the dimethyl esters experimentally by the pulse-heating method. Although, there is no corroborative evidence of their accuracy, we will compare the results of our predictions with the experimental data of Verevkin *et al*. (2006). Table 4 contains the experimental critical properties of the dimethyl esters determined by Verevkin and his co-workers.

Table 4: Experimental critical properties of the dimethyl esters

Dimethyl Ester	Nc	T_c/K(exp.)	P_c/bar (exp.)
dimethyl oxalate	4	639.00 ± 6	40.60 ± 1.20
dimethyl malonate	5	628.00 ± 7	35.30 ± 1.10
dimethyl succinate	6	649.00 ± 7	30.60 ± 0.90
dimethyl glutarate	7	662.00 ± 7	27.70 ± 0.80
dimethyl adipate	8	682.00 ± 7	25.00 ± 0.80
dimethyl pimelate	9	692.00 ± 7	23.70 ± 0.70
dimethyl suberate	10	711.00 ± 7	23.00 ± 0.70
dimethyl azelate	11	723.00 ± 7	NIL
dimethyl sebacate	12	742.00 ± 7	20.80 ± 0.70

Figure 1 compares experimental critical temperatures with values predicted by the method of Lydersen. Most of the data lie within an average relative deviation (ARD) of 12.16%. Fig. 2 compares experimental critical temperatures with values predicted by the method of Constantinou and Gani. An average relative deviation (ARD) of 19.85% was recorded for the data generated. Fig. 3 compares experimental critical temperatures with values predicted by the method of Marrero and Gani. The average relative deviation (ARD) for this method was 13.35%. Fig. 4 compares experimental critical pressures with values predicted by the method of Lydersen. Most of the data lie within a band, with an average relative deviation (ARD) of 2.72%. Fig. 5 compares experimental critical pressures with values predicted by the method of Constantinou and Gani. Most of the data lie within an average relative deviation (ARD) of 13.37%. Figure 6 compares experimental critical pressures with values predicted by the method of Marrero and Gani. Most of the data lie within a band, with an average relative deviation (ARD) of 2.14%.
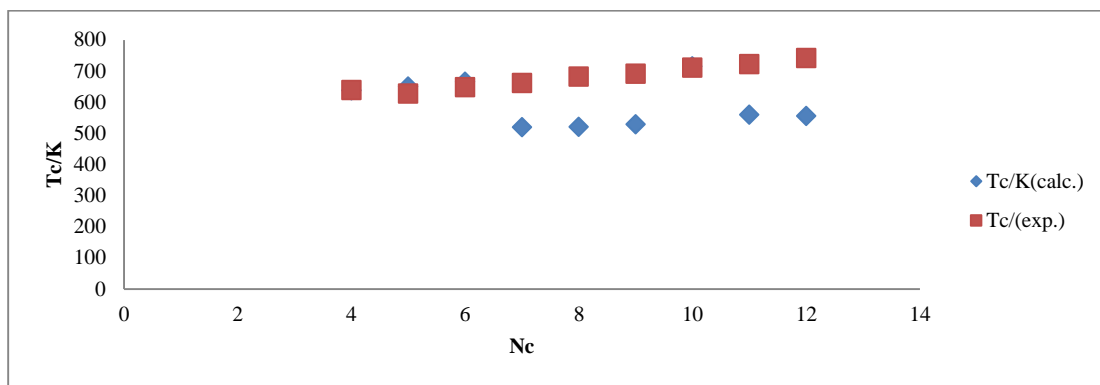
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Figure 1: Deviations of predicted critical temperatures (using Lydersen's method) from experimental data
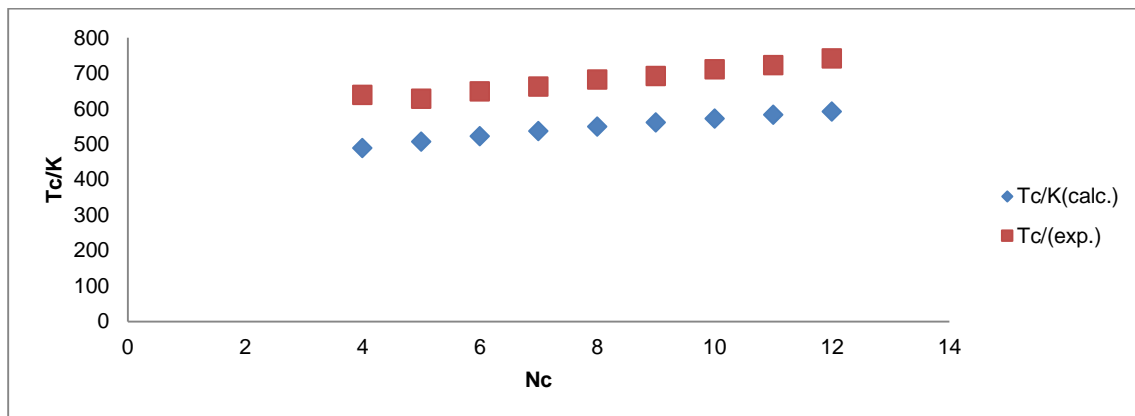

Fig. 2: Deviations of predicted critical temperatures (using Constantinou and Gani's method) from experimental data
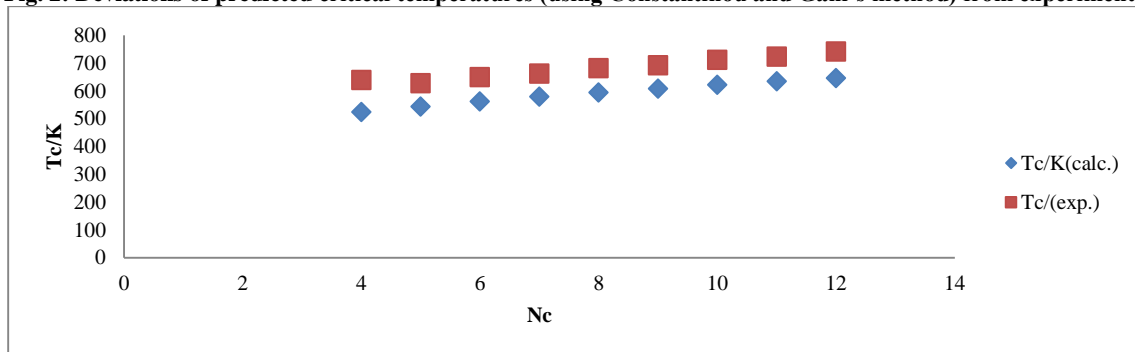

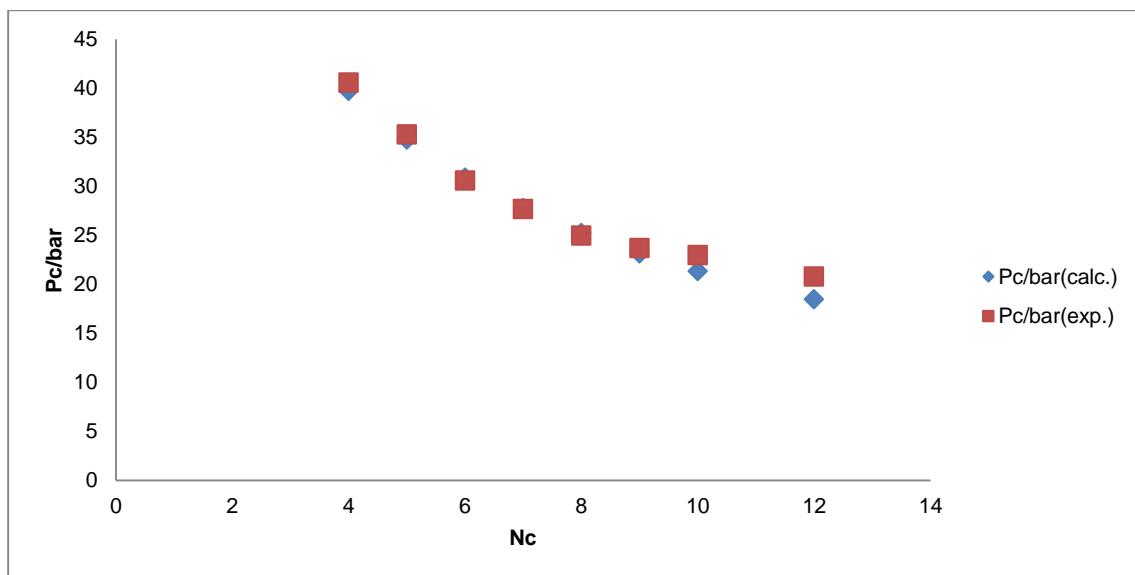**Fig. 3: Deviations of predicted critical temperatures (using Marrero and Gani's method) from experimental data**

Fig. 4: Deviations of predicted critical pressures (using Lydersen's method) from experimental data

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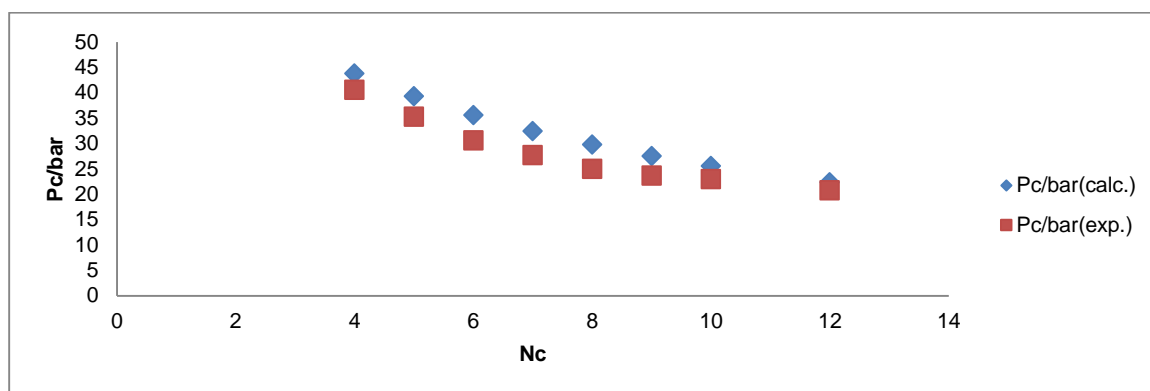
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Fig. 5: Deviations of predicted critical pressures (using Constantinou and Gani's method) from experimental data
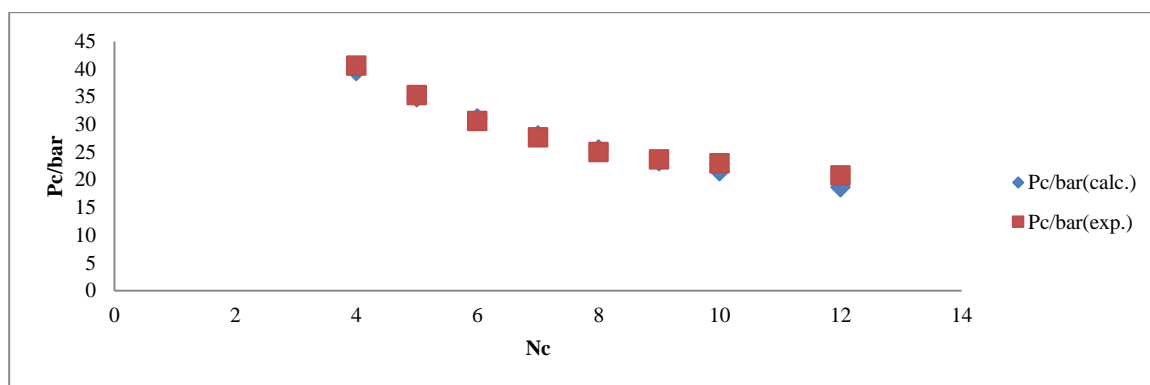

Fig. 6: Deviations of predicted critical pressures (using Marrero and Gani's method) from experimental data

The values for critical temperature and pressure obtained by the Group Contributory methods employed in this study were to an extent in agreement with the findings of Verevkin *et al*., (2006). T_c values obtained by the three methods were below the values sourced from experimental data. This negative deviation becomes more pronounced as the number of carbon atoms increased. However, the methods of Lydersen and Marrero and Gani gave values that were in proximity with experiment than the method of Constantinou and Gani. The P_c values derived from the three methods were also in good agreement with experiment. As was the case with T_c, the methods of Lydersen and Marrero and Gani gave values that were in proximity with experiment than the method of Constantinou and Gani.

Conclusion
The critical temperatures, pressures and volumes of some linear aliphatic dimethyl esters of dicarboxylic acids were predicted using Group Contribution Methods. The results were compared with experimental critical temperatures and pressures of the dimethyl esters. Regrettably, experimental data for critical volume were not available for comparison. The predictions were in good agreement with available experimental data. In general, Lydersen's method and the method of Marrero and Gani yielded better critical properties than the method of Constantinou and Gani. In the case of Lydersen's method, the impute parameter, T_b, which was sourced from experimental data and prediction models for the dimethyl esters, enhanced property prediction. The three stage prediction model of Marrero and Gani makes it a better prediction tool than the earlier two stage version of Constantinou and Gani.

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