

## Prediction of the Thermophysical Properties of Papaya Seed Oil Influencing Solvent Selection Based on the New Group Contribution Model

(Ramalan Sifat Termofizik Minyak Biji Betik Mempengaruhi Pemilihan Pelarut Berdasarkan Model Sumbangan Kumpulan Baru)

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### ABSTRACT

As one of the sustainable food sources, papaya seed oil (PSO) has extraordinary health benefits with unsaturated fatty acids being the main components. In general, the PSO extraction can be accomplished by predetermining the thermophysical properties of the PSO, appropriate use of solvent, and operating conditions. However, the thermophysical properties data of the PSO in the literature are quite scarce, while their quantitative measurements are expensive and time-consuming. For this reason, the group contribution models (GCMs) that have been developed over the last few decades can be essential tools for the estimation of the thermophysical properties of PSO. Moreover, this study also proposes a new GCM to predict PSO thermophysical properties based on its fatty acids composition and validate the accuracy using the experimental data available in the literature. The results showed that the new model has excellent accuracy in estimating the thermophysical properties of PSO at 298.15 K and normal boiling point ( $T_b$ ). The average absolute relative deviation (AARD) for enthalpy of vaporization values at both temperatures were 2.09% and 2.04%, respectively. Meanwhile, the AARD values for molar volume at both temperatures were 0.48% and 0.86%, respectively. Accordingly, the estimated values of the Hansen's solubility parameters and partition coefficients were very close to the experimental data with a distance (D) of 0.21 and AARD of 0.030%. Therefore, this model can be employed to quickly predict the important PSO properties and other its unknown properties based on its molecular structure for its extraction purpose.

Keywords: Extraction; group contribution models; papaya seed oils; thermophysical properties

### ABSTRAK

Sebagai salah satu sumber makanan yang mampan, minyak biji betik (PSO) mempunyai manfaat kesihatan yang luar biasa dengan asid lemak tak tepu sebagai komponen utama. Secara amnya, pengekstrakan PSO boleh dicapai dengan menentukan terlebih dahulu sifat termofizik PSO, penggunaan pelarut yang sesuai dan keadaan pengoperasian. Walau bagaimanapun, data sifat termofizik PSO dalam kepustakaan agak terhad, manakala ukuran kuantitatifnya mahal dan memakan masa. Atas sebab ini, model sumbangan kumpulan (GCM) yang telah dibangunkan sejak beberapa dekad yang lalu boleh menjadi alat penting untuk menganggarkan sifat termofizik PSO. Selain itu, kajian ini juga mencadangkan GCM baharu untuk meramalkan sifat termofizik PSO berdasarkan komposisi asid lemaknya dan mengesahkan ketepatan menggunakan data uji kaji yang terdapat dalam kepustakaan. Keputusan menunjukkan bahawa model baharu mempunyai ketepatan yang sangat baik dalam menganggarkan sifat termofizik PSO pada 298.15 K dan takat didih normal ( $T_b$ ). Purata sisihan relatif mutlak (AARD) untuk entalpi nilai pengewapan pada kedua-dua suhu masing-masing ialah 2.09% dan 2.04%. Sementara itu, nilai AARD untuk isi padu molar pada kedua-dua suhu masing-masing ialah 0.48% dan 0.86%. Sehubungan itu, nilai anggaran parameter keterlarutan dan pekali pemetakan Hansen adalah sangat hampir dengan data uji kaji dengan jarak (D) 0.21 dan AARD 0.030%. Oleh itu, model ini boleh digunakan untuk meramalkan dengan cepat sifat PSO yang penting dan sifat lain yang tidak diketahui berdasarkan struktur molekulnya untuk tujuan pengekstrakannya.

Kata kunci: Minyak biji betik; model sumbangan kumpulan; pengekstrakan; sifat termofizik

## INTRODUCTION

Papaya is a non-seasonal tropical fruit that produces a large amount of seeds (15-20% by weight) (Chielle et al. 2016a). Although many people consider papaya seeds as fruit waste, they are actually edible (Tan 2019). Indeed, the large oil content in papaya seeds (28.2-30.7% by weight) makes them become economically more attractive compared to other plant seeds, such as avocado (1.1-1.6%), olive pomace (8.5-14.9%), and soybean (18-22%) (Sousa et al. 2019). As one of sustainable food sources, papaya seed oil (PSO) contains various

unsaturated fatty acids ( $\pm 77.97\%$ ) (e.g., oleic, palmitic, and linoleic acids) and nutraceuticals (e.g., carotenoids, tocopherols, and phenolics) that provide remarkable health benefits and exhibit the potential of PSO as a functional food material (Kumoro, Alhanif & Wardhani 2020). Table 1 presents the fatty acid compositions of PSO reported in some previous studies, which their values were closely similar. Surprisingly, PSO is comparable to other commercial vegetable oils with high oleic acid, such as canola (75%), safflower (77%), and sunflower (80%) (Yanty et al. 2014).

TABLE 1. The main composition of PSO

CAS No.	Chemical formula	Fatty acid of PSO	Mass Fraction ( $m_x$ )				Mean	Standard Deviation
			Malacrida, Kimura & Jorge (2011)	Samaram et al. (2013)	Yanty et al. (2014)	Chielle et al. (2016)		
544-63-8	$C_{14}H_{28}O_2$	Myristic acid	0.20	0.21	0.30	0.15	0.22	$\pm 0.0624$
57-10-3	$C_{16}H_{32}O_2$	Palmitic acid	16.16	14.90	15.80	16.32	15.80	$\pm 0.6351$
57-11-4	$C_{18}H_{36}O_2$	Stearic acid	4.73	5.21	5.10	4.28	4.83	$\pm 0.4202$
506-30-9	$C_{20}H_{40}O_2$	Arachidic acid	0.38	0.38	0.40	0.27	0.36	$\pm 0.0591$
373-49-9	$C_{16}H_{30}O_2$	Palmitoleic acid	0.27	0.27	0.40	0.00	0.24	$\pm 0.1682$
112-80-1	$C_{18}H_{34}O_2$	Oleic acid	71.30	74.20	73.50	71.52	72.63	$\pm 1.4402$
5561-99-9	$C_{20}H_{38}O_2$	Gondoic acid	0.32	0.42	0.40	0.21	0.34	$\pm 0.0954$
60-33-3	$C_{18}H_{32}O_2$	Linoleic acid	6.06	3.50	4.00	5.06	4.66	$\pm 1.1403$
506-26-3	$C_{18}H_{30}O_2$	$\gamma$ -linolenic acid	0.22	0.17	0.00	0.00	0.10	$\pm 0.1144$
		Other fatty acid compounds	0.36	0.74	0.10	2.19	0.85	$\pm 0.9328$

The PSO can be extracted either through conventional solvent extraction (Soxhlet method) or non-conventional extraction employing ultrasound or/and microwave power (Tan 2019). To obtain an efficient extraction process, a careful selection of an appropriate solvent must be performed. The selection of a suitable solvent can be carried out by predetermining the thermophysical properties of the PSO. Absolutely, thermophysical properties of PSO, such as molecular weight ( $MW$ ), normal

boiling point ( $T_b$ ), enthalpy of vaporization ( $\Delta H_v$ ), molar volume ( $V_m$ ), Hildebrand solubility ( $\delta$ ), Hansen solubility parameters ( $HSPs$ ), and partition coefficient in n-octanol/water ( $\log K_{ow}$ ) being the important ones (Kumoro 2015). These data are needed to determine the extraction conditions and suitable solvent based on the solubility of PSO in various types of solvent. Several thermophysical properties of PSO fatty acids are available in the currently published literature (Yaws 1999). Numerous experimental

data have been digitized in the form of databases, such as the National Institute of Standards and Technology (NIST) (NIST 2021), Chemspider from Royal Society of Chemistry (2021), and Sci-Finder from Chemical Abstracts Service (CAS 2021). However, some other important thermophysical properties, such as  $\Delta H_v$ ,  $V_m$ , and the solubility of certain fatty acids have yet to be understood.

Because measuring the thermophysical properties of a substance is commonly impractical, expensive and time-consuming, estimation of these thermophysical properties using thermodynamic models can be an efficient way to be done. Fortunately, the group contribution models (GCMs), developed in recent decades, have been proven to be suitable for estimating various thermophysical properties of compounds. The main advantage of the GCMs is that they only require the molecular groups contribution data without the need for other input parameters (Su, Zhao & Deng 2017). Other advantages of GCMs are their simplicity and excellent compatibility with various compounds (Fonseca & Cremasco 2021). However, the existing GCMs were obtained randomly from non-linear regression of experimental data from organic or/and inorganic compounds. Thus, to accurately predict the thermophysical properties of PSO fatty acids, all the identified fatty acids must be involved in the model.

Therefore, this study proposed new GCMs obtained from nonlinear regression from tens to hundreds of experimental data on saturated, monounsaturated and polyunsaturated fatty acids. This model can be used to predict the thermophysical properties of  $\Delta H_v$ ,  $V_m$ ,  $HSPs$ , and  $\log K_{ow}$  of PSO based on its fatty acid component. The new GCMs are simple and can be used to estimate the thermophysical properties of fatty acids at various temperatures between 298.15 K to  $T_b$ . In addition, the performance of the new GCMs was also evaluated and compared with the existing GCMs using statistical parameters based on experimental databases. Finally, the GCMs proposed in this study is expected to be satisfactorily for estimating the thermophysical properties of fatty acids in PSO and other vegetable oils.

#### FUNDAMENTAL THEORY PHYSICAL PROPERTIES

The temperature-independent properties of PSO fatty acids, such as normal boiling point ( $T_b$ ), molecular weight ( $MW$ ), and critical temperature parameter ( $T_c$ ), can be obtained from the Yaws, Chemspider and NIST

databases. The  $T_b$  is commonly used to compare different liquid compounds and is an important input parameter for predicting other properties of compounds in various GCMs (Sousa et al. 2019). The  $T_c$  is applied to identify the highest temperature at which the substance can exist as a liquid. This parameter is also required for calculating other properties in several estimation models.

#### ENTHALPY OF VAPORIZATION ( $\Delta H_v$ )

The enthalpy of vaporization ( $\Delta H_v$ ) reflects the difference between the enthalpy of saturated vapor and saturated liquid of a substance at a certain temperature (Abooali & Sobati 2014). Therefore, it is also an important thermodynamic property for predicting  $\delta$  of PSO fatty acids. Although the experimental data of  $\Delta H_v$  for numerous compounds are available in some databases (NIST 2021; Yaws 1999), they are still insufficient for the estimation of  $\delta$  fatty acids at various temperatures. On the other hand, the existing GCMs also need to be evaluated for their accuracy. In this study, a new model was developed to predict the  $\Delta H_v$  value of PSO fatty acids to obtain a model with excellent accuracy.

The  $\Delta H_v$  values of fatty acids can be predicted using GCMs at constant or elevated temperatures, as shown in Table S1 (Appendix). The accuracy of GCMs is strongly affected by the number of compounds involved in the fitting of the group contribution parameters (Benkouider et al. 2014). The new GCM was proposed based on the non-linear regression of experimental data on PSO fatty acids from various literature and databases. In order to obtain the highest coefficient of determination ( $R^2$ ), the exponential, logarithmic, polynomial and other models were fitted with experimental data at various temperature from 298.15 K to normal boiling temperature ( $T_b$ ). Around 120 aliphatic fatty acids data in more than 300 dataset points were utilized in the fitting of a new GCM to predict the  $\Delta H_v$  value of PSO fatty acids. The results of the regression parameters for each fatty acid structure are presented in Table S3 (Appendix).

#### MOLAR VOLUME ( $V_m$ )

Molar volume ( $V_m$ ) is the volumetric space occupied by one mole of a compound or element at a certain temperature and pressure (Moldoveanu & David 2017). This property reflects the structure and intermolecular interactions, which are also closely related to the prediction of  $\delta$  of a compound. GCMs have been widely developed to predict  $V_m$  of various organic or/

and inorganic compounds at a constant and elevated temperatures, as listed in Table S2 (Appendix). The new GCM was developed based on the non-linear regression of experimental data on PSO fatty acids from various literature and databases. Accordingly, the exponential, logarithmic, polynomial and other models were fitted with experimental data to obtain the highest value of coefficient of determination ( $R^2$ ). To allow a wider application, the new GCM for predicting the  $V_m$  of PSO fatty acid was developed as a function of temperatures as presented in Table S2 (Appendix). Similar to GCM in  $\Delta H_v$  prediction, this model also involves 120 aliphatic fatty acids to obtain group contribution parameter values, as presented in Table S3 (Appendix).

#### HILDEBRAND ( $\delta$ ) AND HANSEN ( $HSP_s$ ) SOLUBILITY PARAMETERS

Solvent selection is based on the basic principle that the solute (e.g., PSO) will completely dissolve in the solvent. Therefore, solubility is an essential parameter that can be used to select the appropriate solvent. Solubility parameters, which include  $\delta$  and  $HSP_s$  are widely used to determine the polarity of solvents and solutes, including oil (Stefanis & Panayiotou 2008). The molecular size of a compound significantly affects its solubility where the larger  $V_m$  value will cause a more significant change in its polarity (Kumoro 2015). It is formulated through the following Hildebrand solubility equation (Hildebrand & Scott 1962):

$$\delta = \sqrt{\frac{\Delta H_v - R.T}{V_m}} \quad (1)$$

where  $\Delta H_v$  and  $V_m$  are the enthalpy of vaporization ( $\text{J}\cdot\text{mol}^{-1}$ ) and the molar volume ( $\text{cm}^3\cdot\text{mol}^{-1}$ );  $R$  is the ideal gas constant ( $8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ); and  $T$  is the absolute temperature (K).

Usually, the  $\delta$  parameter is not sufficient enough to describe the molecular behavior of polar compounds and compounds containing hydrogen bonds (H with F, O, or N), (Stefanis & Panayiotou 2008). Therefore,  $HSP$  is used to adequately describe the dispersion ( $\delta_d$ ), polar ( $\delta_p$ ), and hydrogen bonding ( $\delta_{hb}$ ) parameters. Hansen (2007) and Stefanis and Panayiotou (2008) had proposed a predictive model of  $HSP_s$  ( $\text{MPa}^{1/2}$ ) based on GCM. This mathematical expression model was obtained from fitting experimental data of a many compounds. Similar to the previous model, the authors also proposed a new GCM to predict the  $HSP_s$  of PSO fatty acids. The exponential,

logarithmic, polynomial and other models were fitted with experimental data to obtain the highest coefficient of determination ( $R^2$ ). The explicitly, the group contribution to the new model obtained from non-linear regression of experimental data 22 saturated, 13 monounsaturated, and 37 polyunsaturated fatty acids. The regression parameter values are presented in Table S4 (Appendix).

The total  $HSP_s$  can be calculated using the following equation (Hansen 2007):

$$\delta_{HS} = \sqrt{\delta_d^2 + \delta_p^2 + \delta_{hb}^2} \quad (2)$$

In the context of  $HSP_s$ , evaluation of existing or new models may use the term “distance ( $D$ )”. Distance is the difference between two materials (solute-solvent) or two different estimation results (predictive or experimental literature) which are defined by Hansen (2007) as

$$D = \sqrt{4(\delta_d^{pred.} - \delta_d^{lit.})^2 + (\delta_p^{pred.} - \delta_p^{lit.})^2 + (\delta_{hb}^{pred.} - \delta_{hb}^{lit.})^2} \quad (3)$$

#### PARTITION COEFFICIENT n-OCTANOL/WATER ( $\log K_{ow}$ )

The n-octanol/water partition coefficient ( $\log K_{ow}$ ) is defined as the ratio of the equilibrium concentration of a compound in n-octanol to water in a two-phase system (Marrero & Gani 2002). This parameter was used to describe the hydrophilic or hydrophobic properties of the compounds (Meylan & Howard 1995).  $\log K_{ow}$  prediction models have been developed, generally through either atomic or group contribution models. The GCMs previously developed by Meylan and Howard (1995) and Marrero and Gani (2002) were used in this study. In addition, a new model from fitting experimental data on 120 aliphatic fatty acids was also proposed in this study. The new model was built based on the linear regression of experimental data on PSO fatty acids from various literature and databases. The three models are mathematically written as follows:

*Meylan & Howard model*

$$\log K_{ow} = 0.229 + \sum_i N_i \cdot \log K_{ow,i} \quad (4)$$

*Marrero & Gani model*

$$\log K_{ow} = 0.543 + \sum_i N_i \cdot \log K_{ow} (I)_i + \quad (5)$$

$$w \sum_j M_j \cdot \log K_{ow} (II)_j + z \sum_k O_k \cdot \log K_{ow} (III)_k$$

### New Model

$$\log K_{ow} = \sum_i n_i \cdot \log K_{ow,i} \quad (6)$$

where  $\log K_{ow}$  (I),  $\log K_{ow}$  (II), and  $\log K_{ow}$  (III) correspond to contributions to  $\log K_{ow}$  in the first, second, and third levels of groups  $i, j$ , and  $k$  appearing as  $N, M$ , and  $O$  times in a compound.  $\log K_{ow,i}$  for the new model are presented in Table S4 (Appendix).

### MIXING RULES

Kay's rule was employed to calculate the PSO properties from various fatty acid compounds based on the simple molar average (Morad et al. 2000). Based on this rule, the calculation of the critical and thermophysical properties of a mixture formed from many components can be defined as follows:

$$f(x) = \sum_{i=1}^n x_i f(x)_i \quad (7)$$

where  $x_i$  and  $f(x)$  are mole fraction and the specified property of fatty acids. Meanwhile, the mixing rules for the solubility and partition coefficient parameters are calculated using an equation based on the volume fraction ( $\phi$ ) (Kumoro 2015).

$$\delta_{PSO} = \delta_1 \cdot \phi_1 + \delta_2 \cdot \phi_2 + \dots + \delta_n \cdot \phi_n \quad (8)$$

$$\phi_1 = \frac{V_{m,1}}{V_{m,1} + V_{m,2} + \dots + V_{m,n}} \quad (9)$$

where  $\delta_{PSO}$  is PSO solubility.  $\delta_1$ ,  $\delta_2$ , and  $\delta_n$  are the solubility of first, second, and n-th fatty acids.  $V_{m,1}$ ;  $V_{m,2}$ ; and  $V_{m,n}$  are the molar volume of first, second, and n-th fatty acids.

### STATISTICAL ANALYSIS

The accuracy of the thermophysical properties prediction of PSO fatty acids on the existing and the new models against experimental data was evaluated based on the following indicators (Jhamb et al. 2018; Sousa et al. 2019):

*Relative deviation (RD)*, calculated regarding the experimentally measured property values.

$$\%RD = \frac{\text{predicted value} - \text{experimental value}}{\text{experimental value}} \times 100 \quad (10)$$

*Average absolute relative deviation (AARD)*, gives the average relative deviation calculated in absolute values

(ARD) regarding the experimentally measured property values.

$$ARD = |RD| \quad (11)$$

$$AARD = \frac{1}{n} \sum_{i=1}^n ARD \quad (12)$$

n is number of fatty acids contained in papaya seed oil.

## RESULTS AND DISCUSSION

### PHYSICAL PROPERTIES OF PAPAYA SEED OILS

The PSO mainly consists of nine types of fatty acids, with 77.97% being unsaturated (mono and poly) fatty acids (e.g., oleic, linoleic, gondoic, palmitoleic, and -linolenic acids) and the rest are saturated fatty acids (e.g., myristic, palmitic, stearic, and arachidic acids). The number of carbon atoms (CN) and double bonds (DB) distinguishes one from another fatty acid (Sousa et al. 2019). Saturated fatty acids 'fulfilled' with hydrogen on all their carbon atoms. Most saturated fatty acids are straight hydrocarbon chains with an even number of carbon atoms (Rustan & Drevon 2005). The most common monounsaturated fatty acids in biological systems have 14-24 carbon atoms and double bonds with a cis configuration (Berg et al. 2002). It means that the hydrogen atoms on both sides of the double bond are configured with the same direction. In polyunsaturated fatty acids (PUFA), the first double bond can be found between the sixth and seventh carbon atoms of the methyl group, called omega-6 fatty acids (e.g., -linolenic acid). If the first double bond is between the ninth and tenth carbon atoms, it is called omega-9 fatty acid (e.g., linoleic acid). The double bonds in PUFA are separated from each other by methylene groups.

The physical properties of PSO fatty acids are presented in Table 2. These data were obtained from experimental results and databases. The molecular weights of the fatty acid were obtained from the database, which is calculated as the sum of the weights of all atoms that form the respective fatty acid. The molecular weight of PSO is in the molecular weight range of fatty acids with 18 carbon atoms; about 80% of the main constituents are oleic, stearic, and linoleic acids. Molecular weight is an essential property in the characterization of a compound, and it is associated with many properties, especially for the calculation of mixtures in the form of mole fraction ( $x_i$ ).

TABLE 2. Physical properties of PSO

PSO Compounds	CN:DB	Molecular weight (g. mol <sup>-1</sup> ) <sup>(a)</sup>	Mol fraction ( <i>x<sub>i</sub></i> )	Physical Properties	
				<i>T<sub>b</sub></i> (K) <sup>(c)</sup>	<i>T<sub>c</sub></i> (K) <sup>(a)</sup>
Myristic acid	C14:0	228.38	0.0026	592.75	756
Palmitic acid	C16:0	256.43	0.1727	613.75	776
Stearic acid	C18:0	284.48	0.0476	632.55	799
Arachidic acid	C20:0	312.54 <sup>(b)</sup>	0.0032	649.55	823
Palmitoleic acid	C16:1	254.41 <sup>(b)</sup>	0.0026	636.75	789 <sup>(b)</sup>
Oleic acid	C18:1	282.47	0.7208	633.15	781
Gondoic acid	C20:1	310.51	0.0030	699.45	811 <sup>(b)</sup>
Linoleic acid	C18:2	280.45	0.0465	633.75	787
γ-linolenic acid	C18:3	278.43 <sup>(b)</sup>	0.0010	652.65	777 <sup>(b)</sup>
PSO		277.94	1.0000	629.98	781.45

<sup>(a)</sup>(Yaws 1999); <sup>(b)</sup>(NIST 2021); <sup>(c)</sup>(Royal Society of Chemistry 2021)

Another important physical property of PSO is the normal boiling point ( $T_b$ ), which is the temperature at which the vapor pressure of the PSO is equal to one atmosphere. The  $T_b$  of PSO fatty acids are widely available in research databases (Royal Society of Chemistry 2021), which are used as input parameters in the prediction of  $\Delta H_v$  and  $V_m$ . Moreover, the  $T_c$  of fatty acids is also used as an input parameter in predicting their thermodynamic and solubility properties. Most of this data is already available in the database, as summarized in Table 2 (NIST 2021; Yaws 1999). In addition, many researchers have previously proposed  $T_c$  prediction models with the molecular groups and  $T_b$  as the input parameters. Recently, Sousa et al. (2019) proposed a predictive model for estimating the  $T_c$  of fatty acids in biomass, whose values are independent of temperature and easier to use with molecular weight as input parameters. The proposed model provides an excellent predictive value with an AARD of less than 4.6% compared to the NIST database.

#### ENTHALPY OF VAPORIZATION ( $\Delta H_v$ ) OF PAPAYA SEED OILS

The enthalpy of vaporization ( $\Delta H_v$ ) is one of the essential

properties in the prediction of Hildebrand solubility ( $\delta$ ) according to Equation (2). The  $\Delta H_v$  data of several PSO fatty acids at 298.15 K and  $T_b$  are available mainly from the Yaws database (Yaws 1999), as showed in Figure 1. However, no literature completely presents the  $\Delta H_v$  data of fatty acids at various temperatures, which causes serious difficulty to calculate the  $\Delta H_v$  of PSO at different temperatures. Selection of the appropriate predictive model is an alternative effort to obtain the  $\Delta H_v$  value of several fatty acids at a specific temperature, which their experimental data are not presented in the database.

Figure 1 presents the experimental and predicted  $\Delta H_v$  of PSO based on its constituents using various GCMs. Based on the experimental data, the  $\Delta H_v$  values of PSO calculated according to their fatty acid composition were 106.95 and 65.49 kJ.mol<sup>-1</sup> at 298.15 K and  $T_b$ , respectively. In general, at the same temperature, the  $\Delta H_v$  value of PSO increases with increasing carbon chain length and the number of double bonds. From this figure, the predicted  $\Delta H_v$  values of PSO at 298.15 K and  $T_b$  are within the range of its experimental data. The predicted values were influenced by the number of components, family, and temperature involved in

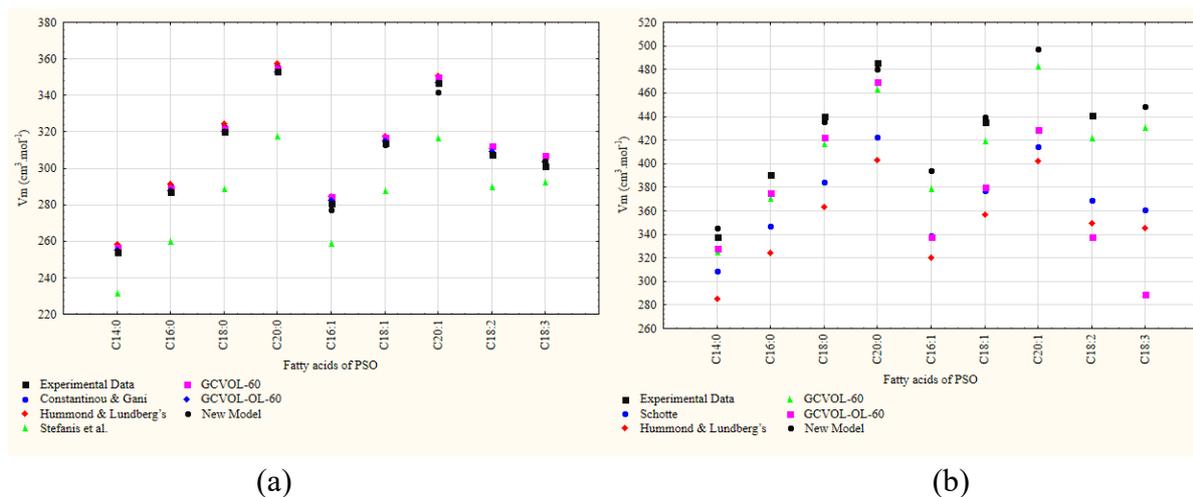


FIGURE 2. Prediction of molar volume ( $V_m$ ) of PSO (a) at 298.15 K (b) at  $T_b$

determining the group contribution parameter values on the GCMs. The statistical analysis used to compare the estimated to the experimental data is the relative deviation (RD) and average absolute relative deviation (AARD) following equation (10) - (12) with detail calculation are presented in Appendix C. Accordingly, the AARD is calculated based on the number of fatty acid components contained in papaya seed oil.

At 298.15 K, a comparison of GCMs with experimental results showed that the new model produced the most excellent  $\Delta H_v$  prediction of PSO (AARD 2.09%), followed by the Oliveira model (2017) with AARD 5.66%. The Oliveira model is intended only to estimate the  $\Delta H_v$  of organic compounds at 298.15 K and is obtained from experimental data on common organic compounds carried out at ambient temperatures. However, at  $T_b$ , the new model and Basarova & Svoboda model (1995) resulted in the best  $\Delta H_v$  of PSO estimation. These observations are corroborated by the calculation of RD and AARD of overall models, as summarized in Table 3. Basarova and Svoboda model (1995) used a set of 307 substance data to calculate the structural contribution parameters consisting of 44 hydrocarbon compounds and 263 hydrocarbon derivatives, the majority of which are halo-derivatives. They reported that the proposed contribution was tested by recalculating the enthalpy of vaporization ( $\Delta H_v$ ) at 298.15 K and at normal boiling point. The mean relative errors were 1.4% and 1.6% for the two value types. On the other hand, the Table 3 also shows that the new model is

the most representative for predicting  $\Delta H_v$  of PSO at two significantly different temperatures with AARD less than 2.1%, respectively. This phenomenon strengthens the presumption that the types of compounds and the number of experimental temperatures significantly affect the value of the group contribution parameters. In fact, the new model proposed in this study uses explicitly experimental data of 120 fatty acids, consisting of 38 saturated, 32 monounsaturated and 50 polyunsaturated fatty acids in the range of 293.15 K to  $T_b$ , respectively. Therefore, the number and composition of the data involved in this study are more representative than other GCMs for predicting the  $\Delta H_v$  of PSO fatty acids.

#### MOLAR VOLUME ( $V_m$ ) OF PAPAYA SEED OILS

Molar volume ( $V_m$ ) is one of the thermodynamic properties that determine the value. A larger value the  $V_m$  indicates a more tenuous the molecular arrangement of a compound, which results in a lower value (see Equation (1)). Figure 2 shows the experimental and predicted  $V_m$  of PSO fatty acids calculated using existing and new GCMs. In general, the  $V_m$  of fatty acids increases with the increase in the number of carbon chains and decreases with the number of double bonds. In addition, the  $V_m$  of fatty acids also increases at high temperatures due to the higher kinetic activity and loose bonds in each fatty acid molecule. As explained earlier, the statistical analysis used to compare the estimated to the experimental data is the relative deviation (RD) and average absolute relative deviation (AARD).

TABLE 3. The relative deviation of the predicted  $\Delta H_v$  of PSO fatty acids at 298.15 K at  $T_b$ 

CN:DB	%RD at 298.15K						
	Basarova & Svoboda (1995)	Tu & Liu (1996)	Kolska et al. (2005)	Ceriani et al. (2013)	Modified Benkouider (2014)	Oliveira (2017)	New Model
C14:0	-11.98	-1.31	1.37	14.40	-11.24	1.55	-1.21
C16:0	-3.93	8.49	9.97	23.42	-0.01	8.45	2.42
C18:0	-1.24	12.44	12.44	25.73	5.50	9.41	0.00
C20:0	4.38	19.86	18.33	32.02	13.95	13.83	0.37
C16:1	-15.82	-2.99	-3.97	7.84	-16.22	-3.32	-3.11
C18:1	-8.28	5.50	4.96	17.41	-7.27	4.10	-1.26
C20:1	-6.25	8.69	6.53	18.88	-3.40	4.31	-5.40
C18:2	-10.21	4.08	2.53	14.75	-14.30	3.65	0.20
C18:3	-17.21	-2.23	-5.19	6.15	-24.77	-2.31	-4.84
AARD (%)	8.81	7.29	7.25	17.84	10.74	5.66	2.09
CN:DB	%RD at $T_b$						
	Joback & Reid (1987)	Basarova & Svoboda (1995)	Tu & Liu (1996)	Kolska et al. (2005)	Ceriani et al. (2013)	Modified Benkouider (2014)	New Model
C14:0	7.79	1.43	-7.70	5.66	14.98	2.53	-0.32
C16:0	10.82	3.80	-3.17	9.20	15.89	10.12	0.55
C18:0	14.15	6.68	2.23	13.01	17.27	18.08	2.46
C20:0	17.44	9.56	7.94	16.76	18.76	25.91	4.66
C16:1	1.99	-5.03	-12.95	-0.42	0.10	-7.47	-3.56
C18:1	9.50	1.37	-4.63	7.48	10.98	2.59	1.03
C20:1	22.00	1.96	-0.41	20.31	8.11	7.10	-0.98
C18:2	9.47	4.21	-5.76	6.52	9.43	-5.84	4.82
C18:3	5.52	-2.51	-12.38	1.78	-0.32	-19.20	0.00
AARD (%)	10.96	4.06	5.65	9.02	10.65	10.98	2.04

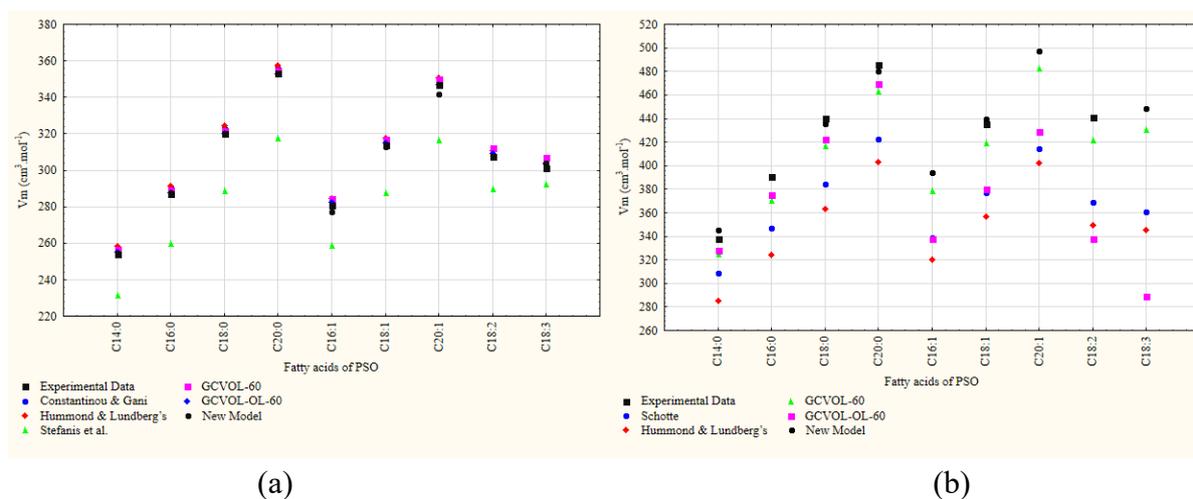


FIGURE 2. Prediction of molar volume ( $V_m$ ) of PSO (a) at 298.15 K (b) at  $T_b$

At 298.15 K, there are five GCMs, namely Constantinou and Gani (1994), Hummond and Lundberg's (Halvorsen, Mammel & Clements 1993), GCVOL-60 (Ihmels & Gmehling 2003), GCVOL-OL-60 (Ihmels & Gmehling 2003), and new model which can produce acceptable  $V_m$  predictions compared to the experimental data (Royal Society of Chemistry 2021; Yaws 1999). Only one model, Stefanis et al. (2005), shows underestimated prediction of  $V_m$ . This result was verified by the calculation of RD and AARD, as summarized in Table 4. Stefanis et al. (2005) model significantly deviated

from the experimental data on saturated fatty acids (RD > 9%), but the deviation decreased with the increasing the number of double bonds with AARD 8.03%. This model uses the principle of indirect  $V_m$  prediction by calculating the specific volume of a compound and was more appropriate for predicting hydrocarbon and aromatic properties (Stefanis et al. 2005). On closer inspection, the GCVOL-OL-60 model (Ihmels & Gmehling, 2003) had the best predictive results among the five existing models with an AARD of 0.32%, followed by the new model with an AARD of 0.48%.

TABLE 4. Relative deviation of the estimated  $V_m$  of fatty acids

CN:DB	%RD at 298.15K						%RD at $T_b$				
	Constantinou & Gani (1994)	Hummond & Lundberg's (1993)	Stefanis et al. (2005)	GCVOL 60 (2003)	GCVOL-OL-60 (2003)	New Model	Schotte (1992)	Hummond & Lundberg's (1993)	GCVOL 60 (2003)	GCVOL-OL-60 (2003)	New Model
C14:0	1.25	1.49	-9.03	0.88	0.44	0.10	-8.74	-15.62	-3.98	-2.84	2.04
C16:0	1.05	1.38	-9.51	0.70	0.22	0.15	-11.34	-17.08	-5.24	-4.05	0.00
C18:0	0.88	1.28	-9.88	0.55	0.03	0.02	-12.64	-17.49	-5.36	-4.11	-1.01
C20:0	0.75	1.20	-10.17	0.43	-0.12	-0.15	-12.99	-17.12	-4.62	-3.29	-1.15
C16:1	1.26	1.33	-7.83	1.25	0.50	-1.22	-	-	-	-	-
C18:1	1.06	1.22	-8.37	1.03	0.27	-0.27	-13.46	-18.05	-3.67	-12.69	0.96
C20:1	0.89	1.13	-8.79	0.84	0.08	-1.48	-	-	-	-	-
C18:2	1.24	1.02	-5.70	1.53	0.51	0.00	-16.46	-20.78	-4.41	-23.49	0.03
C18:3	1.41	0.86	-2.97	2.01	0.74	0.89	-	-	-	-	-
PSO	1.09	1.21	8.03	1.03	0.32	0.48	12.60	17.69	4.55	8.41	0.86

Unfortunately, the prediction of  $V_m$  of PSO fatty acids with GCMs showed less encouraging results at high temperatures ( $T_b$ ). Of the four existing GCMs and new models applied, only GCVOL-60 and the new model have an excellent AARD. In the model proposed by Ihmel and Gmehling (2003), both GCVOL-60 and GCVOL-OL-60 have a low deviation between the estimated results and the experimental data (AARD < 1.1%) at 298.15 K. However, at the normal boiling point, GCVOL-60 has much better performance than the GCVOL-OL-60. These results follow the report of Ihmel and Gmehling (2003), where GCVOL-60 provided simplicity, reliability, and a wider range of applications, suitable for further development.

On the other side, Schotte (1992) stated that the limitations of the number experimental data  $V_m$  at  $T_b$  triggered the regression of the group contribution values not to accurately represent all the expected organic components. Halvorsen, Mammel and Clements (1993) explained that the model proposed by Hummond and Lundberg's is an expanded form of the previous model, which uses an experimental temperature below 354.15 K. A similar phenomenon also occurs in the GCVOL-60 and its extension form (GCVOL-OL-60 model). Several group contribution parameters were adopted from previous studies using a temperature of 200-500 K (Ihmels & Gmehling 2003). Meanwhile, the new model proposed in this study is specifically formed from the non-linear regression of fatty acid (only) experimental data at 298.15 K until each fatty acids boiling point ( $T_b$ ) to obtain the value of the group contribution parameter. Good prediction results from this model illustrate that this model is expected to estimate  $V_m$  from various types of fatty acids in other oil sources.

#### HILDEBRAND SOLUBILITY ( $\delta$ ) OF PAPAYA SEED OILS

Hildebrand solubility ( $\delta$ ) is the most widely used indicator in determining the polarity of solutes and solvents (Kumoro 2015). The solubility of a substance will be maximum if the solute and solvent have a similar  $\delta$  value. The similarity of  $\delta$  causes the intermolecular forces between the solvent molecules and between the solute molecules to have the same strength, and hence, the solvent will be suitable for the respective solute (Stefanis & Panayiotou 2008). If the  $\delta$  of a substance is not available in the database, its value can be predicted as the square root of the cohesive energy density (Equation (1)). Table 5 presents the predictions of  $\delta$  of PSO at 298.15 K and  $T_b$  based on the fatty acid

composition. This prediction involves the previously estimated thermodynamic properties,  $\Delta H_v$  and  $V_m$  of PSO fatty acids. These properties are the best-estimated results of GCM. Based on the facts in the previous section, the new model produces encouraging  $\Delta H_v$  and  $V_m$  predictions involving the PSO fatty acid functional group. Determination of  $\delta$  for fatty acid mixtures was carried out by applying mixing rules based on volume fraction ( $\phi$ ) (Kumoro 2015).

Two factors influence the effect of increasing carbon chain length on the decline of the  $\delta$  value of fatty acids, namely the cohesive energy, which is represented by the enthalpy of vaporization ( $\Delta H_v$ ) and the molar volume ( $V_m$ ). Table 5 shows that the effect of  $V_m$  on  $\delta$  value is more pronounced than that of  $\Delta H_v$ . A more significant change in  $V_m$  than  $\Delta H_v$ , either with increasing the number of carbons or double bonds, causes  $V_m$  to be more pronounced to the shift in the  $\delta$  value. In addition, the  $\delta$  value was also influenced by the temperature at which the solubility is estimated. The  $\delta$  value will decrease with increasing temperature due to the increasing distance between molecules. Based on the new model for  $\Delta H_v$  and  $V_m$  of PSO, the predicted  $\delta$  PSO at 298.15 K and  $T_b$  were 18.34 and 11.90 MPa<sup>1/2</sup>, respectively.

#### HANSEN SOLUBILITY PARAMETERS ( $HSPs$ ) OF PAPAYA SEED OILS

As mentioned before, the  $\delta$  parameter is usually not sufficient to describe the solubility behavior for polar compounds, as well as for compounds containing hydrogen bonding. The reason is that these compounds have three types of intermolecular forces, namely the dispersion ( $\delta_d$ ), polar ( $\delta_p$ ), and hydrogen bonding ( $\delta_{hb}$ ) forces (Stefanis & Panayiotou 2008). Therefore, to increase the prediction accuracy and usefulness of the solubility parameters,  $HSPs$  (partial solubility parameters) have been developed.

The  $HSPs$  of PSO obtained from the predictions based on existing GCMs, new model, and literature are summarized in Table 6. In the context of  $HSPs$ , the 'D' parameter can be used to measure the degree of difference in the solubility of two different substances (solute-solvent) or evaluate the accuracy of the prediction results against the literature data (see Equation (3)) (Batista, Guirardello & Krähenbühl 2015). An example calculation is presented in Appendix C. From this parameter, it can also be seen that the new model proposed in this study provides a better prediction for  $HSPs$  of PSO than the other models ('D' low).

TABLE 5. Prediction of Hildebrand solubility ( $\delta$ ) of PSO at 298.15 K and  $T_b$ 

CN:DB	Hildebrand Solubility of PSO at 298.15 K, (MPa) <sup>1/2</sup>					
	$\Delta H_v^{(a)}$ (kJ.mol <sup>-1</sup> )	$V_m^{(a)}$ (cm <sup>3</sup> .mol <sup>-1</sup> )	Mole (m)	Volume (cm <sup>3</sup> )	Volume fraction ( $\emptyset$ )	$\delta$ (MPa) <sup>1/2</sup>
C14:0	94.39	254.58	0.0009	0.24	0.0022	19.00
C16:0	99.00	287.74	0.0616	17.72	0.1609	18.32
C18:0	102.93	320.36	0.0170	5.44	0.0494	17.71
C20:0	106.18	352.79	0.0011	0.40	0.0037	17.15
C16:1	106.31	277.44	0.0009	0.26	0.0023	19.35
C18:1	108.01	313.04	0.2571	80.49	0.7308	18.36
C20:1	106.18	352.79	0.0011	0.37	0.0034	17.76
C18:2	111.30	307.50	0.0166	5.10	0.0463	18.81
C18:3	113.36	303.88	0.0004	0.11	0.0010	19.10
PSO	106.33	308.72	0.3567	110.14	1.0000	18.34
CN:DB	Hildebrand solubility of PSO at $T_b$ , (MPa) <sup>1/2</sup>					
	$\Delta H_v^{(a)}$ (kJ.mol <sup>-1</sup> )	$V_m^{(a)}$ (cm <sup>3</sup> .mol <sup>-1</sup> )	Mole (mol)	Volume (cm <sup>3</sup> )	Volume fraction ( $\emptyset$ )	$\delta$ (MPa) <sup>1/2</sup>
C14:0	59.11	345.07	0.0009	0.32	0.0021	12.53
C16:0	62.04	391.00	0.0616	24.08	0.1566	12.07
C18:0	65.37	435.91	0.0170	7.40	0.0481	11.74
C20:0	68.87	480.25	0.0011	0.55	0.0036	11.50
C16:1	64.61	394.28	0.0009	0.36	0.0024	12.27
C18:1	67.16	439.53	0.2571	113.02	0.7350	11.87
C20:1	62.69	497.19	0.0011	0.54	0.0035	10.70
C18:2	69.65	441.61	0.0166	7.33	0.0477	12.07
C18:3	68.90	448.76	0.0004	0.16	0.0010	11.89
PSO	66.27	431.02	0.3567	153.77	1.0000	11.90

<sup>(a)</sup>New model proposed in this study

TABLE 6. Prediction of Hansen solubility parameters (*HSPs*) (MPa<sup>1/2</sup>) of PSO at 298.15 K

CN:BD	Hansen Model (2007) (MPa <sup>1/2</sup> )			Stefanis & Panayiotou Model (2008) (MPa <sup>1/2</sup> )			New Model (MPa <sup>1/2</sup> )			References Values (2016) (MPa <sup>1/2</sup> )			Distance (D)		
	$\delta_d$	$\delta_p$	$\delta_{hb}$	$\delta_d$	$\delta_p$	$\delta_{hb}$	$\delta_d$	$\delta_p$	$\delta_{hb}$	$\delta_d$	$\delta_p$	$\delta_{hb}$	HM	SPM	New Model
C14:0	17.45	0.47	2.58	15.74	1.24	5.99	16.27	3.70	6.80	16.30	3.40	6.60	5.49	2.51	0.36
C16:0	17.46	0.42	2.29	15.68	0.96	5.17	16.28	3.41	6.20	16.30	3.40	6.00	5.30	2.85	0.21
C18:0	17.47	0.37	2.06	15.63	0.68	4.35	16.29	3.13	5.60	16.30	3.30	5.50	5.08	3.16	0.20
C20:0	17.47	0.34	1.87	15.58	0.40	3.52	16.30	2.84	5.00	16.30	2.90	5.00	4.67	3.24	0.06
C16:1	17.26	0.45	2.63	15.74	1.01	5.95	16.51	3.42	6.53	16.50	3.40	6.40	5.02	2.86	0.14
C18:1	17.29	0.41	2.36	15.69	0.73	5.13	16.53	3.13	5.93	16.50	3.10	5.70	4.57	2.92	0.24
C20:1	17.31	0.37	2.14	15.64	0.45	4.31	16.54	2.85	5.33	16.60	2.60	5.30	4.12	3.05	0.28
C18:2	17.11	0.44	2.68	15.75	0.79	5.91	16.76	3.14	6.26	16.80	3.10	6.20	4.45	3.14	0.11
C18:3	16.92	0.48	3.01	15.81	0.84	6.70	16.99	3.15	6.58	17.00	3.20	6.50	4.43	3.36	0.10
PSO	17.32	0.41	2.35	15.69	0.77	5.13	16.48	3.18	5.97	16.47	3.16	5.76	4.70	2.92	0.21

Moreover, the relative position of *HSPs* ( $\delta_d$ ,  $\delta_p$ ,  $\delta_{hb}$ ) of PSO and their fatty acid constituents between one and another model can be determined using a 3-D plot, as illustrated in Figure 3. *HSPs* of used frying oils, palm oils, and coconut oils were used to draw the interaction boundary area (sphere), representing the general interaction of vegetable oils. Used frying oils and palm oils spheres are areas that restrict the similarity or interaction of *HSPs* based on the values of  $\delta_d$ ,  $\delta_p$ ,  $\delta_{hb}$ , and  $R_0$  (interaction radius) (Batista, Guirardello & Krähenbühl 2015). It means that other substances outside the sphere have weak interactions with used frying oils and palm oils (not soluble in each other). The *HSPs* 3-D plots of PSO and their constituent fatty acids are in spheres, close to the center coordinates of used frying oil, palm oil, and coconut oil. This condition indicates that the *HSPs* characteristics of PSO are similar to other common vegetable oils. In addition, the 3-D plot can also provide an exact coordinate and distance between the Hansen model (2007), Stefanis and Panayiotou Model (2008), and new model to the reported value (de La Peña-Gil et al. 2016). The coordinates of the new model are closest to the reported value than other models. The advantage

of this model is the uniformity and the large number of compounds involved in predicting *HSPs* for various types of fatty acids. Furthermore, the 3-D spherical plot is also very satisfactory for studying the interaction between solute and solvent, and it can be used to select a suitable solvent for PSO extraction in future studies.

#### PARTITION COEFFICIENT n-OCTANOL/WATER ( $\log K_{ow}$ ) OF PAPAYA SEED OILS

In general,  $\log K_{ow}$  is a quantity that expresses the ability of a solvent to extract a compound and is expressed as the ratio between the equilibrium concentration of the compound in the solvent and the water (Kumoro 2015).  $\log K_{ow}$  also represents the hydrophobicity of the compound (Meylan & Howard 1995). A higher value of  $\log K_{ow}$  indicates the higher concentration of the compound in the octanol (hydrophobic) phase. If the  $\log K_{ow} > 0$ , the compound tends to be more hydrophobic, and vice versa. By studying the hydrophobic or hydrophilic properties of a compound, it will be beneficial to determine the suitable solvent for extracting a specific compound.

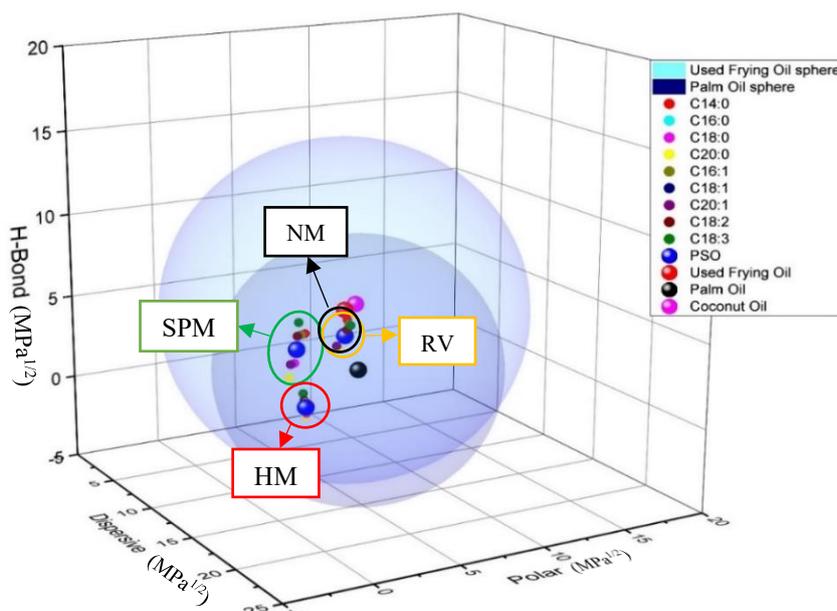


FIGURE 3. The  $HSPs$  ( $MPa^{1/2}$ ) 3-D plot of PSO and common vegetable oils

The  $\log K_{ow}$  value of a compound can be measured from experiments, acquired from databases, or predicted. The statistical analysis used to compare the estimation results with experimental data is the relative deviation (RD) and average absolute relative deviation (AARD), as also used in analyzing the enthalpy of vaporization and molar volume. Table 7 summarizes the  $\log K_{ow}$  values of PSO based on the fatty acid components obtained from the database and the predicted values using existing GCMs and the new model. The accuracy of all models was verified by calculating the average ARD of PSO fatty acids as presented in Table 7. The average ARD values show that Meylan and Howard Model (1995) and the new models have excellent accuracy in predicting the  $\log K_{ow}$  value of PSO with ARD values of 0.539 and 0.030 %, respectively. To determine the parameter group contribution to the estimated  $\log K_{ow}$  value, Meylan and Howard (1995) used 8406 unique organic chemicals. 5257 times fragment  $-CH_3$ , 4630 times  $-CH_2-$ , 2126 times  $-CH=$ , and 547 times  $-COOH$  appeared in determining the group contribution parameters. They stated that the more frequently these groups appear, the lower the deviation from the estimation results.

On the other hand, although the Marrero and Gani (2002) model uses  $\log K_{ow}$  predictions for three levels of

group contribution, it is complex and has a wide variety of organic compounds. Thus, the prediction accuracy is highly dependent on the number of fatty acid compounds involved in determining their group contribution parameters. At the first level, group contributions are composed of simple groups representing various organic compounds but cannot distinguish between isomers and compound proximity. The second level involves organic, polar or nonpolar, medium-sized,  $C_3$ - $C_{10}$ , and aromatic or cyclo-aliphatic compounds. The third level of estimation allows for complex and large heterocyclic properties ( $C_{10}$ - $C_{70}$ ) of polyfunctional acyclic compounds but involves fewer compounds in determining their group contribution parameters.

Then, from the  $\log K_{ow}$  value of PSO ( $\log K_{ow} > 0$ ), it is confirmed that PSO is highly hydrophobic. This value was found to be higher than organic solvents such as benzene (2.13), toluene (2.73), n-hexane (4.0), and n-octane (5.15) (Kumoro 2015). Theoretically, it indicates that organic solvents, such as the aliphatic hydrocarbons, ethers, and esters families are more suitable solvents than water, alcohols, acids, ketones and amines. However, to obtain similar properties and increase the solubility of the solvent to the solute, mixing two or more types of solvents can be carried out.

TABLE 7. Prediction of partition coefficient n-octanol/water ( $\log K_{ow}$ ) of PSO at 298.15K

CN:DB	Partition coefficient n-octanol/water ( $\log K_{ow}$ ) of PSO						
	Database <sup>(a)</sup>	Meylan & Howard Model (1995)	ARD (%)	Marrero & Gani Model (2002)	ARD (%)	New Model	ARD (%)
C14:0	5.980	5.980	0.000	5.318	11.066	5.980	0.003
C16:0	6.960	6.962	0.032	6.218	10.656	6.962	0.034
C18:0	7.940	7.944	0.055	7.118	10.347	7.945	0.058
C20:0	8.930	8.927	0.038	8.019	10.207	8.927	0.036
C16:1	6.750	6.703	0.699	6.249	7.424	6.747	0.044
C18:1	7.730	7.685	0.582	7.149	7.517	7.729	0.010
C20:1	8.710	8.667	0.491	8.049	7.588	8.711	0.017
C18:2	7.510	7.426	1.124	7.269	3.208	7.514	0.052
C18:3	7.300	7.166	1.833	7.389	1.221	7.299	0.021
PSO	7.607	7.571	0.539	7.004	7.693	7.608	0.030

<sup>(a)</sup>(Royal Society of Chemistry 2021)

### CONCLUSIONS

This paper presents a comprehensive study of various existing GCMs and new models for predicting the thermophysical properties of PSO based on its fatty acid composition at 298.15 K and  $T_b$ . Some important temperature-independent properties ( $T_b$ ,  $MW$ , and  $T_c$ ) were collected from the database, while the temperature-dependent properties ( $\Delta H_v$ ,  $V_m$ ,  $HSPs$ , and  $\log K_{ow}$ ) were estimated using the existing GCMs and the proposed model. As expected, the existing GCMs performed well in estimating the  $V_m$ ,  $HSPs$  and  $\log K_{ow}$  values of PSO fatty acids. The newly developed GCM is not only simple to use, but it also demonstrates encouraging accuracy for estimating the temperature-dependent thermophysical properties of PSO fatty acids at various temperatures between 298.15 K to  $T_b$ . Hence, this model offers wide potential applications for the prediction of the thermophysical properties of various types of vegetable oils and animal fat oils that have yet to be explored.

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#### A. Existing and New GCMs

Models	Year	Equation forms
Constant T		
Joback & Reid	1987	$\Delta H_v(Tb) = 15.3 + \sum N_i \cdot H_{v,i}$ <p>where <math>N_i</math> is the number of group contributions and <math>H_{v,i}</math> represents the value of these contributions to the <math>\Delta H_v</math>.</p>
Kolská, Růžička & Gani	2005	$\Delta H_v(298.15 K) = h_0 + \sum_{i=1}^{n_0} N_{h_0,i} \cdot C_{h_0,i} + w \sum_{j=1}^{m_0} M_{h_0,j} \cdot D_{h_0,j} + z \sum_{k=1}^{o_0} O_{h_0,k} \cdot E_{h_0,k}$ $\Delta H_v(Tb) = h_b + \sum_{i=1}^{n_b} N_{h_b,i} \cdot C_{h_b,i} + w \sum_{j=1}^{m_b} M_{h_b,j} \cdot D_{h_b,j} + z \sum_{k=1}^{o_b} O_{h_b,k} \cdot E_{h_b,k}$ <p>In eq., <math>N_{h_0,i}</math> and <math>N_{h_b,i}</math> indicate the number of occurrences in the compounds; <math>C_{h_0,i}</math> and <math>C_{h_b,i}</math> represent the corresponding contributions to the property. <math>M_{h_0,j}</math>, <math>M_{h_b,j}</math>, <math>D_{h_0,j}</math>, and <math>D_{h_b,j}</math> for second-level. <math>O_{h_0,j}</math>, <math>O_{h_b,j}</math>, <math>E</math>, and <math>E_{h_b,j}</math> for third-level.</p>
Oliveira	2017	$\Delta H_v(298.15 K) = 19.55 + \sum_i N_i \cdot C_i$ <p>where <math>N_i</math> is the number of group contributions and <math>C_i</math> represents the value of these contributions to the <math>\Delta H_v</math>.</p>
Function T		
Basařová & Svoboda	1995	$\Delta H_v = A(1 - T_r)^\alpha \exp(-\alpha \cdot T_r)$ <p>with</p> $A = \sum_i v_i \cdot A_i$ $\alpha = \sum_j v_j \cdot \alpha_j$ <p>Where <math>v_i</math> and <math>v_j</math> are the number of group contributions, subscript <math>i</math> and <math>j</math> denotes the type of group contribution; <math>A_i</math> and <math>\alpha_i</math> are the values of these contributions.</p>

Tu & Liu	1996	$\Delta H_v = A(1 - T_r)^{\frac{1}{3}} + B(1 - T_r)^{\frac{2}{3}} + C(1 - T_r)$ <p>where <math>T_r = \frac{T}{T_c}</math>. A, B, and C represent the value of these contributions to the <math>\Delta H_v</math>.</p>
Ceriani, Gani & Liu	2013	$\Delta H_v = 8.3144(-B + C \cdot T) \cdot \left(1 - \frac{T}{T_c}\right)^{\left(\frac{p^{vp}}{P_c}\right)}$ $\ln(p^{vp}) = A + \frac{B}{T} + C \cdot \ln(T)$ $A = \sum_k N_k \cdot (A_{1k} + M \cdot A_{2k}) + (s_0 + N_{cs} \cdot s_1) + \alpha \cdot (f_0 + N_c \cdot f_1)$ $B = \sum_k N_k \cdot (B_{1k} + M \cdot B_{2k}) + \beta \cdot (f_0 + N_c \cdot f_1)$ $C = \sum_k N_k \cdot (C_{1k} + M \cdot C_{2k})$ <p>where <math>N_k</math> is the number of groups <math>k</math> in the molecule, <math>M</math> is the component molecular weight, <math>N_{cs}</math> is the number of carbons of the alcoholic part. <math>N_c</math> is the total number of carbon atoms. <math>A_{1k}</math>, <math>B_{1k}</math>, <math>C_{1k}</math>, <math>A_{2k}</math>, <math>B_{2k}</math>, <math>\alpha</math>, <math>\beta</math>, <math>C_{2k}</math>, <math>s_0</math>, <math>s_1</math>, <math>f_0</math> and <math>f_1</math> are the parameters obtained by regression.</p>
Benkouider et al.	2014	$\Delta H_v = (A - A \cdot T_r + A \cdot T_r^2) + [C_1(1 - T_r)]^B$ <p>with</p> $A = \sum N_i \cdot a_i$ $B = \sum N_i \cdot b_i$ <p><math>C_1</math> is a modified adjustable parameter (<math>C_1 = 1.293 \times 10^{-3}</math>), <math>N_i</math> is the number groups of type <math>i</math>; <math>a_i</math> and <math>b_i</math> are group contribution.</p>
New Model	2022	$\Delta H_v = A + B \cdot \left(\frac{T}{T_c}\right)^N$ $A = \sum n_i \cdot A_i$ $B = \sum n_i \cdot B_i$ $N = \sum n_i \cdot N_i$ <p>where <math>A_i</math>, <math>B_i</math>, and <math>N_i</math> are each component group's contribution values that appear <math>n</math> times. <math>T</math> is the temperature where the <math>\Delta H_v</math> is estimated (K). <math>T_c</math> is the critical temperature of each component.</p>

TABLE S2. GCMs for prediction of molar volume ( $V_m$ )

Schotte	1992	$V_m(Tb) = 0.32L(L - 1) + \sum_j A_j \cdot G_j$ <p>where <math>A_j</math> is the number of groups, <math>G_j</math> is the group contribution for group <math>j</math>, and <math>L</math> is the chain length.</p>
Constantinou & Gani	1994	$V_m(298.15 K) = \sum_i N_i \cdot C_i + \sum_j M_j \cdot D_j$ <p>In eq., <math>C_i</math> and <math>D_j</math> are the group contribution. <math>N_i</math> and <math>M_j</math> denote the number of occurrences of the individual groups in a compound.</p>
Stefanis et al.	2005	$v_{sp}(298.15 K) = \sum_i n_i \cdot F_i + \sum_j m_j \cdot S_j + 1.19155$ $V_m = v_{sp} \cdot MW$ <p>In eq., <math>F_i</math> and <math>S_j</math> are the group contribution. <math>n_i</math> and <math>m_j</math> are the number of occurrences of the individual groups in a compound. <math>v_{sp}</math> is a specific volume of compounds.</p>

		Function T
Halvorsen, Mammel & Clements	1993	For saturated and monounsaturated fatty acids is: $V_m = 16.54C - 6.65D + 26.09 + (0.006C + 0.0085)(T - 293.15)$ For polyunsaturated fatty acids is: $V_m = 16.54C - 6.87D + 26.09 + (0.006C + 0.0085)(T - 293.15)$ where C is the number of carbon atoms, D is the number of double bonds in the fatty acid chain and T is the temperature in K.
Ihmels & Gmehling	2003	$V_m = A_i + B_i T + C_i T^2$ GCMs in the research of Ihmels & Gmehling (2003) are divided into 2, namely GCVOL-60 and GCVOL-OL-60. Where $A_i$ , $B_i$ , and $C_i$ represent the value of these contributions to the $V_m$ .
New Model	2022	$Vm = A + B \cdot \left(\frac{T}{T_c}\right)^N$ $A = \sum n_i \cdot A_i$ $B = \sum n_i \cdot B_i$ $N = \sum n_i \cdot N_i$ where $A_i$ , $B_i$ , and $N_i$ are each component group's contribution values that appear n times. T is the temperature where the $V_m$ is estimated (K). $T_c$ is the critical temperature of each component.

## B. Contributions of simple groups

TABLE S3. Contributions of simple groups to the enthalpy of vaporization ( $\Delta H_v$ ) and molar volume ( $V_m$ )

Contribution of fatty acid groups	$\Delta H_v$			$V_m$		
	$A_i$	$B_i$	$N_i$	$A_i$	$B_i$	$N_i$
-CH <sub>3</sub>	-1023.7	-94.047	0.0558	-24.0453	102.384	0.1918
-CH <sub>2</sub> - or =CH <sub>2</sub>	-0.0338	1.0136	0.0805	0.00039	23.8796	-0.0029
=CH-	-0.2301	-0.0548	0.3365	16.5433	9.3015	0.0286
-COOH	1142.89	-0.0012	0.2809	-54.9822	72.7662	0.1918

TABLE S4. Contributions of simple groups to the enthalpy of Hansen solubility ( $HSP_s$ ) and partition coefficient in n-octanol/water ( $\log K_{ow}$ )

Contribution of fatty acid groups	$HSP_s$			$\log K_{ow,i}$
	$\delta_d$	$\delta_p$	$\delta_{hb}$	
-CH <sub>3</sub>	-0.0966	-0.1273	-0.3330	0.5214
-CH <sub>2</sub> - or =CH <sub>2</sub>	0.0057	-0.1422	-0.3002	0.4911
=CH-	0.1227	-0.1390	-0.1368	0.3834
-COOH	16.2972	5.5293	10.7392	-0.4345

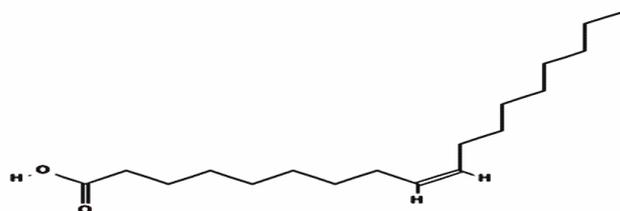
C. Example of application of the group-contribution model to oleic acid (C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>)

FIGURE S1. Chemical structure of oleic acid

(1)  $\Delta H_v$  estimation (Data from Table S3)TABLE S5.  $\Delta H_v$  Characteristic constant estimation

Group contributions	Occurrences, $n_i$	$\Delta H_v$		
		A = $n_i \cdot A_i$	B = $n_i \cdot B_i$	N = $n_i \cdot N_i$
-CH <sub>3</sub>	1	-1023.7	-94.047	0.0558
-CH <sub>2</sub> -	14	-0.4729	14.1909	1.1270
=CH-	2	-0.4602	-0.1095	0.6729
-COOH	1	1142.89	-0.0012	0.2809
$\Sigma$		118.2294	-79.9664	2.1366

Approximation value:

$$\Delta H_v = A + B \left( \frac{T}{T_c} \right)^N$$

At 298.15 K

$$\Delta H_v = 118.2294 + (-79.9664) \left( \frac{298.15}{781} \right)^{2.1366}$$

$$= 108.0121 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\text{Approximation error: } \frac{(108.0121 - 109.3894)}{109.3894} \times 100\%$$

$$= -1.2591\%$$

At T<sub>b</sub>

$$\Delta H_v = 118.2294 + (-79.9664) \left( \frac{633.15}{781} \right)^{2.1366}$$

$$= 67.1594 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\text{Approximation error: } \frac{(67.1594 - 66.4716)}{66.4716} \times 100\% = 1.0346\%$$

(2)  $V_m$  estimation (Data from Table S3)TABLE S6.  $V_m$  Characteristic constant estimation

Group contributions	Occurrences, $n_i$	$V_m$		
		A = $n_i \cdot A_i$	B = $n_i \cdot B_i$	N = $n_i \cdot N_i$
-CH <sub>3</sub>	1	-24.0453	102.384	0.1918
-CH <sub>2</sub> -	14	0.0054	334.3149	-0.0400
=CH-	2	33.0866	18.6031	0.0572
-COOH	1	-54.9822	72.7662	0.1918
$\Sigma$		-45.9355	528.0678	0.4008

Approximation value:

$$V_m = A + B \left( \frac{T}{T_c} \right)^N$$

At 298.15 K

$$V_m = -45.9355 + 528.0678 \left( \frac{298.15}{781} \right)^{0.4008}$$

$$= 313.0398 \text{ cm}^3 \cdot \text{mol}^{-1}$$

$$\text{Approximation error: } \frac{(313.0398 - 313.9000)}{313.9000} \times 100\%$$

$$= -0.2740\%$$

At Tb

$$V_m = -45.9355 + 528.0678 \left( \frac{633.15}{781} \right)^{0.4008}$$

$$= 439.5298 \text{ cm}^3 \cdot \text{mol}^{-1}$$

$$\text{Approximation error: } \frac{(439.5298 - 435.3703)}{435.3703} \times 100\%$$

$$= 0.9554\%$$

(3) *HSPs* estimation (Data from Table S4)TABLE S7. *HSPs* Characteristic constant estimation

Group contributions	Occurences, $n_i$	<i>HSPs</i>		
		$\sum \delta_d$	$\sum \delta_p$	$\sum \delta_{hb}$
-CH <sub>3</sub>	1	-0.0966	-0.1273	-0.3330
-CH <sub>2</sub> -	14	0.0802	-1.9903	-4.2025
=CH-	2	0.2453	-0.2780	-0.2735
-COOH	1	16.2972	5.5293	10.7392
$\Sigma$		16.5261	3.1337	5.9302

Approximation value:

$$\delta_{HS} = \sqrt{\delta_d^2 + \delta_p^2 + \delta_{hb}^2}$$

$$\delta_{HS} = \sqrt{(16.5261)^2 + (3.1337)^2 + (5.9302)^2} = 17.8353 \text{ MPa}^{1/2}$$

Approximation error (Distance) in Eq. (3)

$$D = \sqrt{4(\delta_d^{pred.} - \delta_d^{lit.})^2 + (\delta_p^{pred.} - \delta_p^{lit.})^2 + (\delta_{hb}^{pred.} - \delta_{hb}^{lit.})^2}$$

$$D = \sqrt{4(16.5261 - 16.5)^2 + (3.1337 - 3.1)^2 + (5.9302 - 5.7)^2} = 0.2385$$

(4)  $\log K_{ow}$  estimation (Data from Table S4)TABLE S8.  $\log K_{ow}$  Characteristic constant estimation

Group contributions	Occurences, $n_i$	$\log K_{ow,i}$
-CH <sub>3</sub>	1	0.5214
-CH <sub>2</sub> - or =CH <sub>2</sub>	14	6.8756
=CH-	2	0.7669
-COOH	1	-0.4345
$\Sigma$		7.7292

Approximation value:

$\text{Log } K_{ow}$  of oleic acid = 7.7292

Approximation error: =  $\frac{(7.7292 - 7.73)}{7.73} \times 100\% = -0.0099\%$ .