A study of relative dissociation energy through electro-optics effect as a potential tool for evaluation of cooking oil quality

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Abstract. The electro-optics effect is a potential tool to observe and evaluate different oil quality. In this research, we study relative dissociation energy through the electro-optics effect to evaluate vegetable oil quality. Some vegetable cooking oil samples with different quality were placed in an external potential difference between parallel plates to obtain the electro-optical characteristics by measuring the polarization change using red pointer laser (650 nm). The empirical values of dissociation energy was obtained by fitting experimental data of the average polarization changes per unit potential difference with Lenard-Jones potential formula under the assumption that the interaction between molecules is a Vander Waals interaction. The results show that the average change in polarization is proportional to Lenard-Jones potential energy. An important result showed that a good oil quality is indicated by relatively high dissociation energy. Reducing the oil quality leads to increasing relative dissociation energy. This provides electro-optics as a very potential method in differentiating various cooking oil qualities and new perspective of interacting linear polarized light with oil molecules.

1. Introduction

So far, many researchers have worked a lot in developing various equipment systems to evaluate the quality of cooking oil. Various methods and various quality parameters have been carried out and developed in an effort to obtain the best way of testing the quality of oil, not only during the cooking or heating process but also after the heating process and the level of oil quality degradation during the storage process [1-17]. In our understanding, the various quality parameters as well as the variety of equipment systems or methods used are too complex and should be summarized into a single quality parameter by a simple method or equipment; therefore, it would be an interesting challenge to find a single quality parameter with the simplest method.

Since 2011, we have developed an electro-optical method for evaluating the quality of cooking oil by measuring changes in light polarization after passing through an oil sample and found that this method is relatively simplest [18-24]. The level of oil quality measured by changes in the polarization angle not only provides information on the natural properties of cooking oil but also provides a new understanding of oil quality and also provides an alternative understanding of the interaction of light with cooking oil molecules [21-24]. We surprisingly found that this electro-optical method has great potential as a method for evaluating oil quality and yielding the single most probable parameter of oil quality [21]. The change in polarization on the other hand indicates the nature of cooking oil and in an external electric field known as the electro-optical effect, the change in the average polarization of each
change in the electric potential difference shows the potential energy state of the triglyceride molecules according to the Lenard-Jones potential. In the previous research, in case for canola oil [21] it was found that the electro-optical method is very potential for the evaluation of oil quality. This method provides a new perspective that in an external electric field, the change in average polarization per potential difference is the result of Van der Waals interactions between molecules and leads to a single quality variable for cooking oil in the form of relative dissociation energy. In this paper, we use the electro-optics method to study and obtain the relative dissociation energy in soybean oil and coconut oil.

2. Methods

The samples were soybean oil and coconut oil and were assumed as standard oils and in good condition according to the date of expiration. The samples were heated in an oven at around 100 °C with a heating duration of 2, 4, 6, and 8 hours for each sample. The change of polarization due to potential difference was measured by using a pair of the polarizer with a light source of a red pointer laser with \( \lambda = 650 \) nm. The linear polarized incoming light was assumed to be homogeneous in the interval of polarizer angle \( \varphi=0^\circ \) to \( 90^\circ \), and in a selected case, we chose mode angle at \( \varphi=0^\circ \) and \( \varphi=90^\circ \) to be compared. The data acquisition and detail of measurement were similar to the previous report [21].

We proposed that molecular interaction between triglyceride molecules during applying potential difference obeyed Van der Waals interaction as previously reported [21], and therefore the Lenard-Jones potential energy can be described by equation

\[
V_{L,J} = V_m \left( \frac{R_m}{R} \right)^{12} - 2 \left( \frac{R_m}{R} \right)^{6},
\]

where \( V_m \) is maximum dissociation energy, \( R \) molecular distance, and \( R_m \) maximum molecular distance where the \( V_{L,J} = -V_m \) takes place. According to the hypothesis, the Lenard-Jones potential was proportional to the average change in polarization per unit potential difference as \( V_{L,J} = \alpha \Delta \theta \Delta V \), where \( \alpha \) is proportional parameter and can be regarded as unity. The experimental data of relative potential energy \( \Delta \theta \Delta V \) was obtained by measuring the change of polarization \( \Delta \theta \) divided by the applying potential difference \( \Delta V \) in the range of 0-9 kV from high DC voltage. These experimental values were then plotted against potential difference, with the definition that the increment of molecular distance was proportional to the increment of potential difference through \( R = (\Delta V + a)/b \), where \( a \) and \( b \) are scale parameters, and it yields

\[
\frac{\Delta \theta}{\Delta V} = E_0 + E_m \left( \frac{\Delta V + a}{b} \right)^{12} - 2 \left( \frac{\Delta V + a}{b} \right)^{6},
\]

in which \( E_0 \) is intercept value, \( E_m \) relative dissociation energy and \( \zeta_m \) relative maximum molecular distance. We plotted \( \Delta \theta \Delta V \) vs. \( \Delta V \) and the empirical values \( E_0, E_m \) and \( \zeta_m \), were obtained by fitting the equation (2) with experimental data.

3. Results and discussion

The results show that the change of polarization \( \Delta \theta \) through electro-optics is polynomial function of potential difference \( \Delta V \) that shows a nonlinear response of sample to the external field from electro-optics effect for all samples. This behaviour is still in agreement with our previous studies [18-24]. In more deeply analyzed, the applying of the potential difference to the sample is none other than placing the oil molecules in an excited state. This is indicated by the position of the polarization change which increases quadratically with the increase in the potential difference. Likewise, heating the sample results in a larger polarization change. This means that it also provides a greater potential so that the molecules tend to become asymmetrical. The results of previous studies also indicated that heated samples then placed in an electric field underwent a greater change in polarization [21, 22]. The heated sample means the quality decreases as indicated by the increase in the angle of polarization. Giving a potential difference to the sample in principle does not change the quality of the sample, but actually, it proportionally informs how the light interacts with the electric dipole. Figure 1 is an example of electro-
optics data for soybean oil at $\varphi = 0^\circ$ as a representative sample. All samples actually also show similar results as in figure 1.

**Figure 1.** The change in polarization is polynomial against potential difference for soybean oil at heating times 0 h and 8 h. Other samples (not shown) also show similar curves.

**Figure 2.** The experimental data of relative potential energy as a function of potential difference at heating time 0 h and 8 h for soybean oil. All samples also show identical graphs but not shown here.

Figure 2 representatively provides experimental data of relative potential energy $\Delta \theta / \Delta V$ vs. the potential difference $\Delta V$ for soybean oil at angle $\varphi = 0^\circ$ and for heating time 0 h and 8 h. All samples actually also show similar results, as shown in figure 2.

Figure 3 is an example comparison of experimental data and the theoretical formula of equation (2) for soybean oil before heating at mode angle $\varphi = 0^\circ$.

**Figure 3.** The fitting experimental data and theoretical formula to obtain empirical values of $E_0$, $E_m$, and $R_m$. The graph is shown only for soybean oil before heating at angle $\varphi = 0^\circ$. 
From the assumption, the value $\Delta \theta$ is related to the potential energy of the triglyceride molecule while applying potential difference $\Delta V$. The average value of $\Delta \theta/\Delta V$ is experimental data (black dot) that represents relative potential energy (in a unit of $^\circ$/kV). The theoretical formula of equation (2) is represented by red dashed line; it seems that the experimental data is in accordance with the theoretical data. The curves in Figure 3 also apply to coconut oil samples for all heating treatments and angle modes $0^\circ$ and $90^\circ$.

Table 1 and 2 depict the empirical values of $E_0$, $E_m$, and $\zeta_m$ for soybean and coconut oil at a various heating time and mode angle $\phi = 0^\circ$ and $\phi = 90^\circ$.

For both of soybean oil and coconut oil (table 1 and 2) the value $E_m$ decreases by increasing heating time. This indicates that the relative dissociation energy decreases as oil quality reduces after heating. The decreasing $E_m$ is simultaneously accompanied by increasing relative maximum molecular distance $\zeta_m$, and this is also in agreement to the previous study of canola oil [21]. The mode angle $\phi = 0^\circ$ and $\phi = 90^\circ$ for soybean oil leads the same $E_m$ indicating that the orientation of triglyceride molecules is almost the same as it interacts with linear polarized light at the mode angles. Whereas for coconut oil the orientation of molecules is not the same as polarized linear light interacts with these molecules at the mode angle $\phi = 0^\circ$ and $\phi = 90^\circ$, which is indicated by different values $E_m$ at both angles. If it is true that $E_m$ reflects as single oil quality variable, we can say that the quality of coconut oil is relatively temporarily better than soybean oil at this special condition. Because soybean and coconut oil were examined at the same condition and time, and so to obtain these characteristics values of all various cooking oils it is very important to be conducted in the same time and condition. The value $E_m$ seems to be complemented by $\zeta_m$, so that here it is possible that a single parameter value can be chosen either $E_m$ or $\zeta_m$, only. The intercept value $E_0$ reflects the initial condition of the sample before applying the electric field, and it should be in accordance with the natural polarization or initial optical activity of the sample.
If we insert the whole empirical values from tables 1 and 2 into equation (2), we obtain the relative model of Lenard-Jones potential of the samples. Fig 4 describes the relative potential energy of soybean oil at heating time 0 h and 8 h at mode angle of the polarizer $\varphi = 0^\circ$ and $\varphi = 90^\circ$. It seems that the relative potential energy is the same for both angles, indicating the similar orientation of the molecules.

**Figure 4.** The relative potential energy against potential difference for soybean oil at heating time 0 h and 8 h at mode angle $0^\circ$ (left) and $90^\circ$ (right).

In other hand, fig 5 expresses the relative potential energy for coconut oil at the same condition. The relative potential energy is obviously different for both angles, indicating the dissimilar orientation of the molecules, i.e., at angle $90^\circ$, the asymmetric triglyceride molecules are more dominant than at $0^\circ$.

**Figure 5.** The relative potential energy against potential difference for coconut oil at heating time 0 h and 8 h at mode angle $0^\circ$ (left) and $90^\circ$ (right).
molecules increases indicating that the quality of the oil decreases. The basic explanation of the relation between dissociation energy and oil quality can be accommodated base of Firdausi et al. [21]. During the heating process, the triglyceride molecules can undergo several processes, namely oxidation, polymerization, etc., that usually releases free radicals, free fatty acids, and so on. Therefore the remaining triglyceride molecules tend to be more asymmetric than symmetric molecules. As a result, it is easier to be polarized as it interacts with light. In principle, any disturbance that causes a reduction in oil quality leads to the increase of asymmetric molecules. And if it is applied to external potential difference, the sample is placed in additional potential energy. The interaction of a linear polarized light with the sample in this certain condition reflects Van der Waals interaction between molecules. The average change in polarization per unit potential difference is amazingly proportional to the Lenard-Jones potential. This new perspective, as already mentioned in the previous study [21] gives some opportunities in the future. The electro-optics effect provides not only a potential tool for evaluation of cooking oil quality but also it can be further developed to study molecular interaction for other nonpolar molecules.

4. Conclusions
The use of the electro-optical effect in cooking oil is identical to conditioning the sample in the Lenard-Jones potential energy system. The average value of the change in polarization per unit of the electric potential difference applied to the sample is proportional to the Lenard-Jones potential energy. The increase in potential difference is equivalent to increasing the distance between molecules so that the interactions between molecules can be considered as Van der Waals interactions. The relative dissociation energy was reduced with the decrease in the quality of cooking oil. As a single oil quality parameter, this method can further applied to various other cooking oils and can be developed to investigate other nonpolar molecules.

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