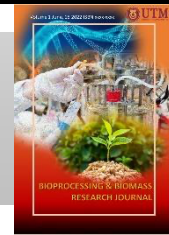




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Research Article

Simulation on Heat Distribution in Oil Palm Fruit Mesocarp during Thermal Hydrolysis of Triacylglycerols

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ABSTRACT

Palm oil industry is a major contributor to Malaysia's economy. Crude palm oil (CPO) extraction involves the digestion of the oil palm fruit mesocarp where thermal hydrolysis of triacylglycerols (TAGs) is crucial for the oil yield and quality. This study aims to develop a comprehensive 2D-asymmetric time-dependent model using COMSOL Multiphysics® for simulating heat distribution during thermal hydrolysis of TAGs and investigating its impact on CPO extraction under varying steam temperatures within a time frame of 90 min. The temperatures of the steam applied are in the range of 90 °C to 100 °C. Simulation results demonstrate a strong correlation between heat distribution and oil yield, providing valuable insights for process optimization. From the result, it can be concluded that the time required for the fruit mesocarp to attain equilibrium temperature is around 60 minutes. The findings also underscore the significant role of temperature in influencing oil extraction efficiency. The maximum molar concentration of the oil extracted is around 35.7 mol/m³ at around 28 °C (301 K) and the minimum molar concentration of the oil extracted is around 28.0 mol/m³ at around 100° C (373 K). This research demonstrates the potential of advanced modelling techniques to drive sustainable efficient palm oil production practices.

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INTRODUCTION

The plantation development of oil palm has been accelerated through large-scale investments and recorded an increase from 5.74 million hectares in 2016 to 5.81 million hectares in 2017. This development has contributed to the acceleration of palm oil production which is in line with the substantial market demand and benefits Malaysia economically (Amiri et al., 2012). According to the research, it stated that oil palm serves as the primary source of vegetable oil globally, contributing approximately 40 % of total production. Southeast Asia is responsible for 88% of global CPO production, with the remaining portion produced in Sub-Saharan Africa and the Americas (Volk et al., 2018).

The palm oil industry constitutes a significant foundation of Malaysia's economy and contributes substantially to its Gross Domestic Product (GDP) through the production of CPO and a wide range of oleochemical derivatives. Despite the industry's economic significance, there are several areas for efficiency and sustainability development in the palm oil milling process, particularly in the digestion stage (Chew et al., 2021).

During this process, the mesocarp of palm fruit is subjected to heat treatment by the injection of hot steam to facilitate the separation of oil from the nuts.

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This is because the heat distribution directly influences the degree of hydrolysis of TAGs which in turn affects the yield and quality of the CPO. Hence, it is necessary to address this concern to ensure the process of extraction of palm oil can be carried out efficiently.

It is found that there is insufficient predictive model for assessing the heat distribution of the hydrolysis of TAGs in the digester during the extraction of palm oil. Recent research has predominantly focused on developing predictive models for the sterilization process occurring in the sterilizer (Asha Embrandiri, 2013). Additionally, the degree of hydrolysis of TAG (oil) will be influenced by the heat treatment on the palm fruits in the digester. The implementation of different temperatures will influence the yield of oil extracted (Etsu, 2019). This is because heat plays an important role in macerating the mesocarp from the kernel and rupturing the oil-carrying cells for the preparation of the oil extraction. During the process, fruit-mashes will absorb water from the surrounding steam, which immediately achieves saturated condition. The increment of the water absorbed into the mesocarp will ease the liberation of oil from the porous and the water then occupies the vacant space. This hydrolysis process contributes to the accumulation of free fatty acids (FFA) due to lipase activity which will impact the quality of the extracted oil. Upon bruising, lipase activity in the mesocarp of palm fruit will be activated, particularly during handling and processing, leading to the accumulation of FFA in the fruit. FFA is a critical quality index of CPO and significantly influences the commercial value. Ineffective sterilization process which is responsible for the high percentage of unstripped bunches (USB) and contributes to partial inactivation of lipase, leading to enzymatic hydrolysis of CPO in subsequent unit operations such as in this case which occurred in the digester unit (Awang, 2016). Therefore, a thorough investigation and evaluation of the impact of the heat distribution on the hydrolysis of TAG in the digester is essential to optimize the process and ensure high-quality palm oil production.

This study aims to address this gap by developing a comprehensive heat distribution model using COMSOL Multiphysics to simulate the thermal hydrolysis of TAGs within the mesocarp and validate it with literature data. The second objective of this study is to simulate the effect of temperature on the yield of oil extracted during the digestion process through the developed model.

Here, the similar method has been used by Shehu et al. (2019a) which is the simulation of heat penetration in palm fruitlets during the thermal treatment process using COMSOL Multiphysics. However, in this research, the investigation of the heat penetration process was performed for the sterilization process during the palm oil mill processing. The temperature used for conducting the simulation were 35 °C, 40 °C, 45 °C, 50 °C, 60 °C and 70 °C for a time frame of 100 minutes. This finding provides insight into improving sterilization efficiency in the palm oil extraction.

The scope of this study includes employing COMSOL Multiphysics for simulation and incorporating an ellipsoid geometry to represent the mesocarp based on the mass transfer, heat transfer and chemical reaction. Besides that, simulation with varying temperatures within the range of 90 °C to 100 °C on the yield of the oil extracted from the mesocarp will be carried out by using the developed model.

METHODOLOGY

Digestion Process Set-up for Fruit Mesocarp

To better model the digestion process set-up fruit mesocarp, the suitable geometry and parameters of the mesocarp were collected from the literature search. According to Yunus et al. (2015) and Shehu et al. (2019a), the most suitable geometry for simulating the shape of the mesocarp of the palm fruit was identified.

The simulation of heat distribution during thermal hydrolysis of TAG in the digester was conducted by using COMSOL Multiphysics. Table 1 was the summary of the parameters that will be required for modelling the geometry during simulation. Figure 1 presents the flowchart detailing the development of the simulation for this study.

Table 1 Model geometry in 2D axisymmetric

Suitable geometry for simulating the palm fruit	
Mesocarp (Outer layer)	Length: 40.00 mm
	Width: 25.00mm
	Thickness: 20.00 mm
Kernel (Inner layer)	Length: 35.96 mm
	Width: 20.15 mm
	Thickness: 17.11 mm

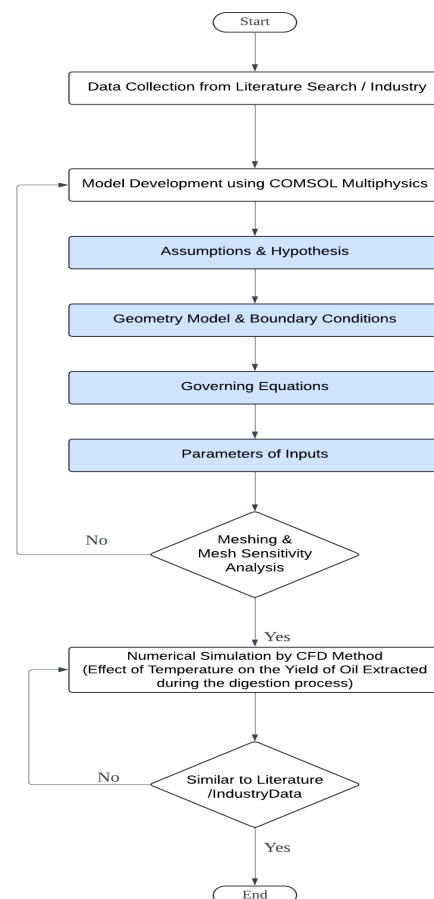


Figure 1 The flowchart of the simulation

Assumptions and Hypotheses

To perform mathematical modelling, several assumptions were established for simplifying the development of the mathematical model. The assumptions were shown below:

- Heat transfer was distributed uniformly on the fruit mesocarp within the digester.

- (b) Minor components (e.g., vitamin E, carotenoids, phytosterols, etc.) were ignored.
- (c) The hot steam used to heat the fruit was pure water.
- (d) Geometry used to construct the shape of palm fruit was assumed to be ellipsoid.
- (e) Heat loss from the wall of the digester to the surrounding was negligible.
- (f) The fibrous mesocarp was homogeneous and isotropic during heating.
- (g) The thermophysical properties of the water and oil including density, viscosity and specific heat capacity were assumed to be constant.

Boundary Conditions

The entering of the mass flux of water onto the fruit surface led to the increase in water content. For the surface of fruit that was in contact with hot steam, the boundary condition for mass transfer of water could be indicated by the below equation:

$$n(D_w \Delta C_w) = k_w(C_{bw} - C_{fw}) \quad (1)$$

where n was the mole fraction of entering water content, D_w was the diffusivity coefficient of water (m^2/s), C_w was the concentration of entering water content (mol/m^3), k_w was the mass transfer coefficient for water (m/s), C_{fw} was the water content of fruit (mol/m^3), C_{bw} was the water content surrounding the liquid (mol/m^3) which was the same as unity.

Furthermore, the decrease in oil content occurred when the mass flux of oil was liberated to the surrounding water. The boundary condition for the mass transfer of oil was:

$$n(D_o \Delta C_o) = k_o(C_{fo} - C_{bo}) \quad (2)$$

where D_o was the diffusivity coefficient of oil (m^2/s), C_o was the concentration of oil content in fruit (mol/m^3), k_o was the mass transfer coefficient for water (m/s), C_{fo} was the water content of fruit (mol/m^3), C_{bo} was the oil content surrounding the water (mol/m^3) which was equivalent to 0.

The boundary condition of heat transfer on fruit surface in contact with water was:

$$n(k_f \Delta T) = h(T_{wv} - T_f) + D_w C_{pw} \Delta C_w T - D_o C_{po} \Delta C_o T \quad (3)$$

For symmetry, mass and heat transfer was derived as:

$$\begin{aligned} -n(D_w \Delta C_w) &= 0, \text{ for water} \\ -n(D_o \Delta C_o) &= 0, \text{ for oil} \\ -n(k_f \Delta T) &= 0, \text{ for heat transfer} \end{aligned}$$

Mass Transfer and Component Balance

During the digestion process, there were two components involved in the mass transfer which were water and oil. In this process, water would be absorbed into the fruit mash whereas the oil would be liberated from the fruit. According to Yunus et al. (2015), it could be assumed that the mass transfer which included moisture diffusion or water transfer occurs only in radial direction and D_w was uniform at any coordinate points. Hence, the rate of water transfer into the fruit could be represented by the equation:

$$\frac{\partial C_w}{\partial t} = D_w \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_w}{\partial r} \right) = D_w \frac{\partial^2 C_w}{\partial r^2} + 2 \frac{\partial C_w}{r \partial r} \quad (4)$$

where D_w was defined as the diffusivity coefficient of water which diffused into the mesocarp of the fruit.

Similarly, the rate of oil released within the fruit could be expressed as:

$$\frac{\partial C_o}{\partial t} = D_{wo} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_o}{\partial r} \right) = D_o \frac{\partial^2 C_o}{\partial r^2} + 2 \frac{\partial C_o}{r \partial r} \quad (5)$$

where D_o was defined as the diffusivity coefficient of oil which released from the mesocarp of the fruit.

Heat Transfer in Solid

In this process, two different types of heat transfer took place which were convection and conduction. The convection heat transfer occurred from hot water (steam) to the mesocarp, while the conduction heat transfer happened within the mesocarp. The overall heat transfer within the mesocarp was contributed by the fluid movement of water and oil during the digestion process. Hot water which was condensed steam was the only heat source for the digestion process. When the steam jacket surrounding the wall of the digester supplied energy (hot steam) directly into the digester, the energy was released into the air, and some penetrated the fruit mesocarp (Hosseini et al., 1992). The convective heat transfer equation could be expressed as:

$$q = h(T_{wv} - T_f) \quad (6)$$

where q was the convective heat flux (W/m^2), h was the heat transfer coefficient (W/m^2K), T_{wv} was the temperature of hot steam (K) and T_f was the initial temperature of fruit (K).

Based on Yunus et al. (2015), the equation of the heat transfer that occurred in the mesocarp was modified as follows:

$$\rho_f C_{pf} \frac{\partial T}{\partial t} + \rho_w C_{pw} u_w \Delta T - \rho_o C_{po} u_o \Delta T = \Delta(k_f \Delta T) \quad (7)$$

where ρ was the density of the component (kg/m^3), C_p was the specific heat capacity ($J/kg K$) and k was the thermal conductivity ($W/m K$), u was the fluid velocity (m/s), T was the temperature (K), and t was the time (s). The subscript f represented the mesocarp whereas w and o were water and oil respectively. The negative sign in the equation showed that the heat was released from the mesocarp during the liberation of oil.

Parameters of Inputs

In this study, there was a lot of data that needed to be collected including the schematic reaction of thermal hydrolysis of TAG, the operational temperature range of the digester, suitable geometry for simulating the palm fruit and the equations used for modelling. These data were collected from different research papers. The information regarding the schematic reaction of thermal hydrolysis of TAG was retrieved from various literature (Wae-hayee et al., 2022; Marisa, 2021).

The operational temperature range of the digester was obtained. The most suitable geometry for simulating the shape of real palm fruit was identified from the research paper by Yunus et al. (2015) and Shehu et al. (2019b). From Etsu (2019), equations for developing the model were acquired. The molecular weight, density and other relevant

data of the compounds involved were also gathered from various reliable sources (Yunus et al., 2015; Othman et al., 2022; Grassini & Slingerland, 2024; Chandra et al., 2020). **Table 2** summarized all the parameters needed for the simulation.

Table 2 Summary of the parameters required for simulation

Range of temperatures of the hot steam (water), T_b	90 °C, 92 °C, 94 °C, 96 °C, 98 °C and 100 °C
Temperature of the fruit, T_f	28 °C
Pressure in the digester	1 atm
Heat transfer coefficient	250 W/m ³ K
Molecular weight	Water: 18 g/mol Oil: 22 g/mol Free fatty acid: 288.424 g/mol Glycerol: 95.072 g/mol
Density	Water: 997 kg/m ³ Oil: 993 kg/m ³ Free fatty acid: 841.2 kg/m ³ Glycerol: 1260 kg/m ³
Viscosity of water	8.5×10^{-4} Ns/m ²
Thermal conductivity	Water: 0.62 W/mK Oil: 0.347 W/mK
Heat capacity	Water: 4.180 kJ/kgK Oil: 2.816 kJ/kgK
Diffusivity	Water: 2.0×10^{-9} m ² /s Oil: 1.24×10^{-7} m ² /s

RESULTS AND DISCUSSION

Geometry and Meshing

To conduct simulation of a system or process, meshing can be considered as a vital method in producing accurate simulation. For constructing a mesh, it needs the coordinate locations of the points of the elements in space that illustrate the geometry of certain shapes (Ilyas et al., 2022). Apart from that, the appropriate number of elements that formulate the overall shape of the fruit mesocarp is also required (Shehu et al., 2019a).

This simulation was conducted by utilizing the ellipsoid geometry that represents the actual shape of the palm fruit. **Figure 2** shows two-dimensional (2D) geometry of ellipsoid created in the axisymmetric 2D plane with the mesh to model the oil palm fruit mesocarp.

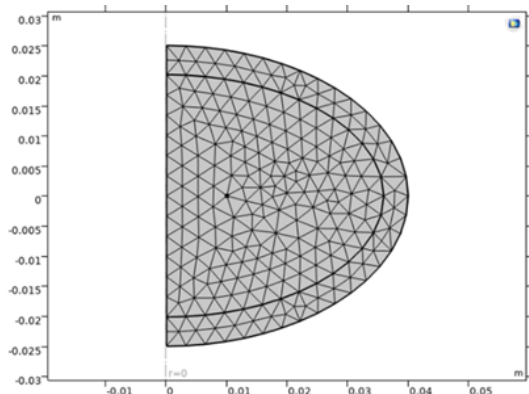


Figure 2 Two-dimensional (2D) geometry of ellipsoid created in the axisymmetric 2D plane with the mesh

Figure 3 shows cut points from coordinates (35,0) to (40,0). These cut points corresponded to different depths of

mesocarp at which CPO was extracted during the thermal hydrolysis of TAGs.

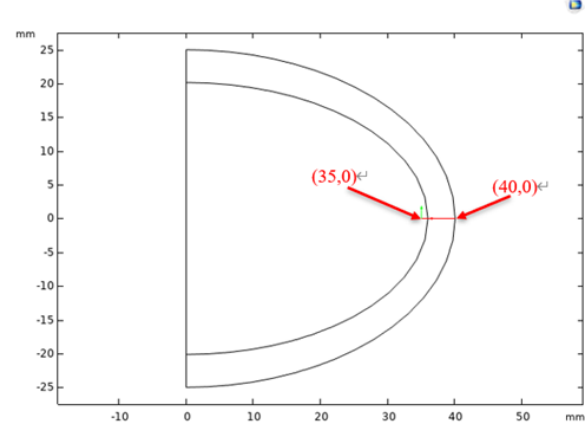


Figure 3 Cut points from coordinates (35,0) to (40,0). These cut points corresponded to different depths of mesocarp

Validation of the Simulated Model

The simulated results from this model were analyzed through one-dimensional plots (1D plots) which included line graphs and point graphs in COMSOL Multiphysics. **Figure 4** illustrates the point graph of the simulated molar concentration of CPO extracted against the digestion time for various cut points within the palm fruit. The graph revealed that all the cut points exhibit a similar trend with the molar concentration decreasing exponentially over the digestion time. This trend reflected the thermal hydrolysis process took place in breaking down the TAGs, leading to a progressive reduction in the extractable CPO. After approximately 60 minutes, the molar concentration approached nearly constant values across all the cut points. This implied that the thermal hydrolysis process had reached equilibrium.

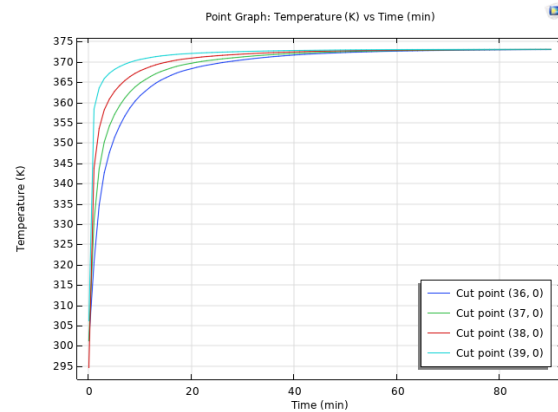


Figure 4 Heat distribution temperature profiles predicted by the current model in this work

In **Figure 4**, the simulated heat distribution profiles demonstrated a steady increase in temperature over time until a thermal equilibrium was achieved. This aligned with the trend observed in Shehu et al. (2019a) where the temperature stabilized after certain periods. By comparing the simulated model in **Figure 4** to the heat distribution profiles reported by Shehu et al. (2019a), it was evident that the heat transfer characteristics, including the rate of temperature rise and the stabilization phase matched previously validated data. In addition, the simulated model correctly captured the heat distribution dynamics expected

during thermal hydrolysis of TAGs. This included the initial rapid temperature increase due to the heat input and the temperature eventually reaching the stable state when thermal equilibrium was achieved. The simulated heat distribution model as depicted in **Figure 4** shows good agreement with the results retrieved from [Shehu et al. \(2019a\)](#). This indicated that the model accurately replicates the thermal behaviour during thermal hydrolysis of TAGs in fruit mesocarp, supporting its validity for further predictive and optimization purposes.

Temperature Profiles during Thermal Hydrolysis of Triacylglycerols in Fruit Mesocarp

Figure 5 presents surface plots of temperature distribution within an oil palm fresh fruit during the digestion process in the digester at different times: 0, 5, 10, 30, 60 and 90

minutes. The color scale ranges from 301 K (dark blue) to 310 K (red), indicating how the temperature evolves within the object over digestion time. At the beginning (0 minute), the fruit is uniformly cool (~301 K). When digestion progresses, heat gradually penetrates from the outer surface inward. At 5 and 10 minutes, the outer layers begin to heat up while the core remains cool, indicating a strong temperature gradient. By 30 and 60 minutes, the heat has moved deeper into the fruit and the core temperature increases significantly. At 90 minutes, the temperature is more evenly distributed throughout the fruit, suggesting that thermal equilibrium is nearly reached. This temperature rise supports effective oil extraction, as heat softens the fruit and facilitates oil release from the nut during the digestion process.

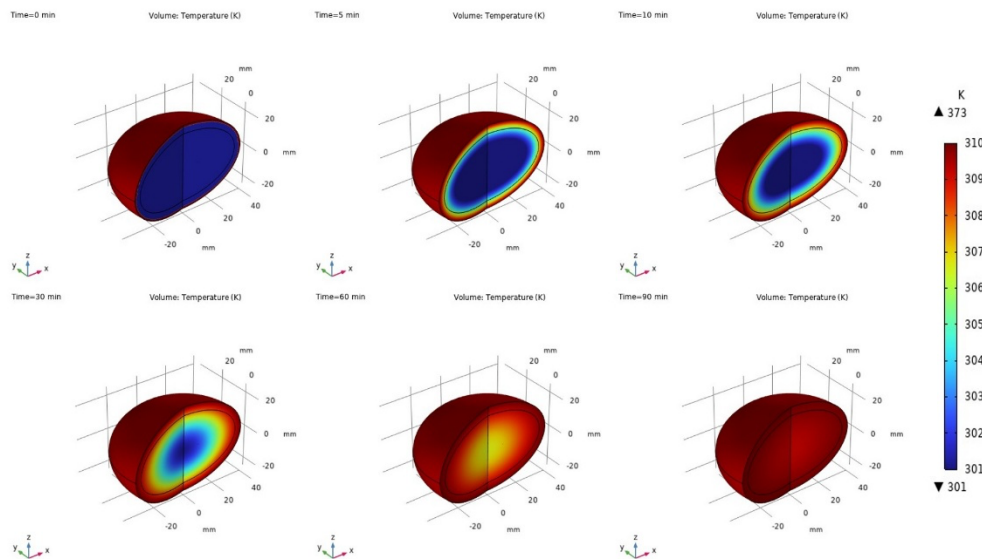


Figure 5 Surface plots of temperature predicted at 0, 5, 10, 30, 60 and 90 minutes

Based on **Figure 6**, the simulation of heat distribution within the mesocarp during the digestion process was carried out at different steam temperatures starting with 28 °C (301 K) to 100 °C (373 K). The objective of this simulation was to see the uniformity of the heat distribution in the mesocarp that was undergoing process in the digester. The heating process was conducted continuously. To perform the simulation, it was assumed that at any time, the temperature of the mesocarp would be higher than that of the kernel.

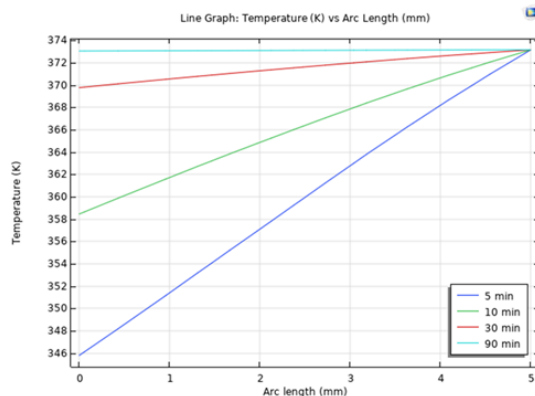


Figure 6 1D plot of the simulated temperature profile at different digestion times

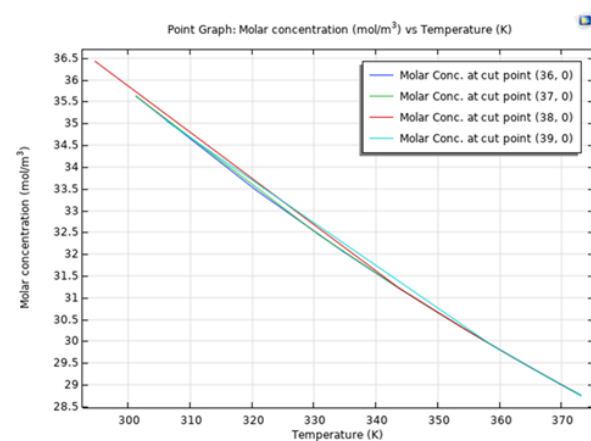


Figure 7 Point graph of the simulated CPO molar concentration profile at different temperatures within time frames of 90 min

Figure 7 illustrates the variation in molar concentration of CPO as a function of temperature. The graph revealed a maximum molar concentration of approximately 35.7 mol/m³ at 28 °C (301 K) and a minimum concentration of around 28.0 mol/m³ at 100 °C (373 K). The initial molar concentration exceeding 35.7 mol/m³ suggests oil extraction occurring prior to the simulated initial set temperature

(28 °C). Therefore, the analysis was initiated at the corresponding molar concentration at 301 K.

From the above graph, all the lines exhibit a negative slope. This demonstrated an inverse relationship between temperature and extracted oil concentration. This trend was expected, as elevated temperatures generally enhance extraction efficiency due to increased reaction kinetics, facilitating the breakdown of cell walls and oil release from the mesocarp. Notably, the highest molar concentration was observed at the cut point (38,0) around 290 K. This phenomenon can be attributed to the depletion of readily extractable triacylglycerols in the mesocarp at previous temperatures. As previously discussed, the oil yield at point (39,0), should be the highest as compared to point (38,0) as point (39,0) is closer to the mesocarp surface. However, the observed reduction in the oil yield at point (39,0) suggests potential oil losses from the mesocarp surface which is represented by point (39,0) during the processing. Since the oil losses took place at the surface, thus, more oil could be extracted from this area (38,0) compared to (39,0) (Shehu et al., 2019b; Mohd Nadzim et al., 2020).

CONCLUSION

The 2D-asymmetric time-dependent heat transfer simulation model has been successfully developed and validated by using literature data. This model successfully simulates the heat distribution during thermal hydrolysis of triacylglycerols within fruit mesocarp and CPO yield at different steam temperatures that correspond to objectives. From the result, it can be concluded that the time required for the fruit mesocarp to attain equilibrium temperature is around 60 min. The temperature near the surface of the mesocarp (39,0) is higher than the temperature at the kernel surface (36,0). Therefore, the heat penetration of heat into fruit mesocarp is dependent on the time and depth for the heat to penetrate. The findings also underscore the significant role of temperature in influencing oil extraction efficiency. The maximum molar concentration of the oil extracted is around 35.7 mol/m^3 at around 28 °C (301 K) and the minimum molar concentration of the oil extracted is around 28.0 mol/m^3 at around 100 °C (373 K). A comparative study between the factors influencing oil extraction rate (OER), other factors that affect the amount of CPO extracted from the digester, the impact of alternative heating methods, such as microwave heating for studying the thermal hydrolysis of TAG within the mesocarp and the influences of enzyme-catalyzed hydrolysis should be carried out in the future.

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Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper

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