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ANALYTICAL METHOD IMPROVEMENT, FORMATION AND MITIGATION OF 2-MCPD, 3-MCPD ESTERS AND GLYCIDYL ESTER IN PALM OIL-CONTAINING FOODS DURING BAKING PROCESS

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By

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Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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Chair: Prof. Tan Chin Ping, PhD
Faculty: Food Science and Technology

Based on the recent European Food Safety Authority Journal 2016, monochloropropanediol (MCPD) ester and glycidyl ester (GE) are critical contaminants predominantly found in palm oil and palm-based food products. MCPD ester is regarded as a nongenotoxic carcinogen, while GE is a genotoxic carcinogen. It is important to improve the current analysis method (with rapid method) and study the formation and mitigation of MCPD ester and GE in baked goods. In this study, it is aimed to evaluate the analysis method (GC-MS/MS and FTIR), formation and mitigation of the formation of 3- and 2-MCPD esters and GE in related baking products and during the baking process. The experiment was divided into four parts. First, the difference in the performance between selected ion monitoring (SIM) and multiple reaction monitoring (MRM) detection mode was assessed. In MRM mode, the limit of detection (LOD) of 3- and 2-MCPD ester was 0.01 mg/kg while the limit of quantification (LOQ) was 0.05 mg/kg. In addition, the limit of detection (LOD) and the limit of quantification (LOQ) of GE were 0.024 and 0.06 mg/kg, respectively. MRM mode showed better repeatability in area ratio and recovery with relative standard deviation (RSD %) < 5% for 2- and 3-MCPD ester. Quantification of 22 food samples using MRM mode showed higher repeatability and reliability compared to SIM, which fluctuated as high as 50% RSD. Second, a baking process was simulated using commercial margarine (control), palm olein, palm mid-fraction, and soft and hard stearin, baked at different temperatures (160, 180 and 200 °C) for 20 min. The results showed soft stearin and palm olein delivered a similar volume, surface color, and texture to the finished product compared to the control. An elevated baking temperature significantly ($p<0.05$) increased the hardness and chewiness, and lowered the springiness of the finished products. The content of MCPD esters from the cake samples was insignificant ($p>0.05$) throughout the experiment, but GE was significantly degraded ($p<0.05$) when a baking temperature of 200 °C was used. Third, palm olein and soft stearin were fortified with antioxidants, BHA, rosemary and tocopherol at single dosage (200 mg/kg) and in combinations (BHA at 200 mg/kg with rosemary or tocopherol at 400, 800 and 1200 mg/kg). Electron spin resonance spectrometry measurement showed that antioxidant was effective to reduce the radical formation. MCPD esters and GE were significantly lower ($p<0.05$) when a higher concentration of natural antioxidants was used. Antioxidants were effective to inhibit oxidation, as well as formation of free fatty acid and unstable 1,2-diacylglycerol. Finally, a rapid prediction of MCPD ester and GE was performed using Fourier transform infrared (FTIR) spectroscopy coupled with chemometrics analysis. The results showed a consensus model was able to predict MCPD ester ($R^2 = 0.91$) and GE ($R^2 = 0.94$) at high accuracy. Among the established individual models, cubist and random forest models performed better to predict MCPD ester, while random forest and neural network model performed equally to predict GE. In conclusion, MCPD esters and GE quantification performed optimally using MRM detection; baking temperature strongly affected the quality and GE content of baked goods; antioxidant in combination was able to control oxidation and MCPD ester and/or GE formation; and finally, a consensus model served as a rapid alternate analysis method in MCPD esters and GE predictions.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia
Sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

PENAMBAHBAIKAN KAEDAH ANALISIS, PEMBENTUKKAN DAN PENGURANGAN 2-MCPD, 3-MCPD ESTER DAN GLISIDIL ESTER DALAM MAKANAN MENGANDUNGI MINYAK SAWIT SEMASA PROSES PEMBAKARAN

Oleh

GOH KOK MING

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Pengerusi: Prof. Tan Chin Ping, PhD
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Berdasarkan Jurnal *European Food Safety Authority* pada tahun 2016, monokloropropandiol (MCPD) ester dan glisidil ester (GE) merupakan bahan pencemar yang critikal dalam minyak sawit ataupun makanan terkandung bahan minyak sawit. MCPD ester ialah bahan karsinogenik dan GE ialah karsinogenik yang bersifat genotoksik. Kajian ini merangkumi penambahbaikan cara analisis, kajian tentang pembentukan, dan pengurangan 2-, 3-MCPD ester dan GE dalam sistem pembakaran kek. Kajian dibahagikan kepada empat bahagian utama. Dalam kajian pertama, prestasi antara *selected ion monitoring* (SIM) dan *multiple reaction monitoring* (MRM) telah dinilai. Had pengesanan (LOD) untuk 3-, dan 2-MCPD ester serendah 0.01 mg/kg dan had kuantifikasi (LOQ) serendah 0.05 mg/kg telah dicapai. Tambahan, GE mempunyai nilai LOD dan LOQ pada nilai 0.024 dan 0.06 mg/kg masing-masing. MRM menunjukkan kebolehulangan dalam nisbah kawasan puncak komatogafi dan pemulihan dengan sisihan piawai relatif (RSD %) < 5%. Kuantifikasi dalam 22 sampel makanan membuktikan bahawa MRM memberi kebolehulangan dan sisihan piawai yang rendah berbanding dengan perubahan sisihan piawai dengan cara analisa SIM sebanyak 50 %. Dalam kajian kedua, satu sistem pembakaran kek disimulasikan dengan menggunakan marjerin (kawalan), minyak sawit olein, pecahan minyak sawit, sawit stearin lembut dan keras sebagai lemak dalam resipi kek. Suhu bakar di ketuhar adalah 160, 180 dan 200 ℃ dengan masa bakar selama 20 min. Keputusan kajian menunjukkan bahawa minyak sawit olein dan sawit stearin lembut boleh menghasilkan kek yang mempunyai isipadu, warna permukaan dan teksur yang sama dengan kumpulan kawalan. Apabila suhu dinaikkan ke 200 ℃, kekerasan dan kekenyalan kek meningkat dan penurunan keanjalan kek yang ketara ($p<0.05$). GE bersifat tidak stabil dan turut berkurang apabila suhu bakar meningkat. Dalam kajian ketiga, penambahan antioksidan (BHA, rosemary dan tokoferol) pada kepekatan 200 mg/kg ke dalam sampel minyak sawit olein dan stearin sawit lembut telah dilakukan. Selain itu, kombinasi antara BHA (200 mg/kg) dengan

rosemary atau tokoferol (kepekatan 400, 800 and 1200 mg/kg) juga dilakukan. Keputusan dari resonansi spin elektron (ESR) menunjukkan kandungan radikal adalah berkurangan dalam sampel berantioksidan. Kepekatan MCPD ester dan GE juga lebih rendah secara ketara ($p<0.05$) apabila kepekatan antioksidan yang digunakan adalah lebih tinggi. Penambahan antioksidan dalam sampel minyak berkesan untuk mengurangkan pengoksidasian, asid lemak bebas dan 1,2-diasilgliserol yang tidak stabil. Dalam kajian keempat, cara analisis menentukan jumlah MCPD ester dan GE dengan cara FTIR bersama dengan kimometrik telah dihasilkan. Keputusan daripada model konsensus berjaya menentukan MCPD ester (R^2 =0.91) dan GE (R^2 =0.94) dengan ketepatan tinggi. Antara model yang dihasilkan, ramalan jumlah MCPD ester lebih baik dengan menggunakan model kubist dan hutan rawak. Ramalan jumlah GE adalah lebih baik dengan menggunakan model hutan rawak dan model rangkaian saraf. Kesimpulannya, kuantifisakasi MCPD ester dan GE lebih optima dengan menggunakan pengesanan MRM; suhu membakar kek mempengaruhi kualiti dan kandungan GE dalam sampel; antioksidan secara kombinasi boleh mengawal proses oksidasi dan pembentukan MCPD ester dan/atau GE; akhirnya, model konsensus adalah cara analisa alternatif untuk menentukan jumlah MCPD ester dan GE.

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I certify that a Thesis Examination Committee has met on 3 May 2019 to conduct the final examination of Goh Kok Ming on his thesis "Analytical Method Improvement, Formation and Mitigation of 2-MCPD, 3-MCPD Esters and Glycidyl Ester in Palm Oil-Containing Foods During Baking Process" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

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LIST OF ABBREVIATIONS

2-MCPD	2-chloropropane-1,3-diol
3-MCPD	3-chloropropane-1,2-diol
AOCS	American Oil Chemist Society
ATR	Attenuated total reflection
avNNET	Average neural network
BHA	Butylated hydroxanisole
CD	Conjugated dienes
CE	Collision energy
CT	Conjugated trienes
DAG	Diacylglycerol
EDX	Energy dispersive X-ray
EFSA	European food safety authority
ELSD	Evaporative light scattering detector
ESR	Electron spin resonance
FFA	Free fatty acid
FTIR	Fourier transform infrared spectrometer
GC	Gas chromatography
GE	Glycidyl ester
HPLC	High performance liquid chromatography
HVP	Hydrolysed vegetable protein
LOD	Limit of detection
LOQ	Limit of quantification
MAG	Monoaclyglycerol

MBPD	Monobromopropandiol
MCPD	Monochloropropandiol
MRM	Multiple reaction monitoring
MS	Mass spectrometry
nnet	Neural network
PBA	Phenylboronic acid
PLSR	Partial least square
RBD	Refined, bleached and deodorized
RF	Random forest
RMSE	Root mean square error
RSD	Relative standard deviation
SG	Savitzky-Golay
SIM	Selected ion monitoring
SNC	Standard normal variate
TAG	Triaclyglycerol
TQMS	Triple quadrupole mass spectrometry

CHAPTER 1

INTRODUCTION

1.1 General Overview

Monochloropropane-1,2-diol (MCPD) is a food processing contaminant initially found in hydrolyzed vegetable protein (HVP) during the late 1970s (Baer, de la Calle, & Taylor, 2010; Velisek, 1979). MCPD and the ester form were eventually found in refined vegetable oils as a potentially harmful contaminant. In addition, glycidyl ester (GE) is another contaminant found in refined vegetable oils which is coexists with MCPD (Cheng, Liu, Wang, & Liu, 2017). At present, the presence of MCPD and GE in processed food, especially food containing palm oil as one of the ingredients, is an aggressively discussed topic. 3-MCPD is accessed as a nongenotoxic carcinogen, while glycidol is a genotoxic carcinogen (Bakhiya, Abraham, Gurtler, Appel, & Lampen, 2011). Although 2-MCPD, as the isomer of 3-MCPD, has limited supporting toxicological data, the potential harmful effects are considered equal to the harmful effects of 3-MCPD (EFSA, 2016).

Commonly, 3- and 2-monochloropropane-1,2-diol are derivatives of glycerol. According to the recent ESFA journal 2016 released on 3 March 2016, with the title "Risk for human health related to the presence of 3- and 2-monochloropropanediol (MCPD), and their fatty acid esters, and glycidyl fatty acid ester in food", the assessment of over 7,175 occurrence data has shown that palm fats and oils have the highest MCPDs and GE compared to other refined vegetable fats and oils (Wallace et al., 2016).

Since the palm oil industry is one of the important industries in Malaysia, and the application of refined, bleached and deodorized (RBD) palm oil in the food processing industry is broad, there is a need to investigate the relationship between derivative products of RBD palm oil and the formation of these unwanted contaminants in related products.

In terms of the analysis method, the detection of MCPDs and GE can be categorized as direct and indirect methods. The direct methods usually involve liquid chromatography with a mass spectrometer detector (LC/MS), which does not require intensive sample preparation (Hori et al., 2012). However, indirect methods are favored by the literature most of the time due to reproducibility, although indirect methods often require extensive derivatization skills and tedious sample preparation and purification (Garballo-Rubio, Soto-Chinchilla, Moreno, & Zafra-Gomez, 2017; Hamlet et al., 2011). Currently, three indirect methods (official methods) using gas chromatography with mass spectrometric detection (GC/MS) have been established by the American Oil Chemists' Society (AOCS). To quantitate the amount of 3- and 2-MCPD as well as GE, AOCS Method 29a-13 is commonly used. Despite the existing analytical methods, the application of Fourier-transform infrared (FTIR) spectrometry is seen as a potential method to detect the presence of these contaminants in current studies. FTIR requires minimal sample preparation to serve as a rapid detection or quantitation method (H. Ayvaz & Rodriguez-Saona, 2015).

Formation of MCPD esters and GE are usually directly related to the heating processes during refining as well as food production. To the best of our knowledge, MCPD esters and GE formation during food processing, for example, frying is well discussed in the literature (Aniolowska & Kita, 2016; Dingel & Matissek, 2015; Y. H. Wong et al., 2017). In addition, in baking, as one of the commonly used heat processes to treat food products, the relationship between formation of MCPD ester and/or GE and baking processes should be studied. Formation of MCPD esters and GE has been studied in the baking process for biscuits (Mogol, Pye, Anderson, Crews, & Gokmen, 2014) and the storage conditions (Sadowska-Rociek & Cieślik, 2016). Bakery goods, especially cakes or biscuits, require the use of fats or oils as the shortening. Cakes, as the subject of interest in the current study, are a popular product with good organoleptic properties. A cake batter consists of fats, sugar, eggs and flour that create finished product with a light and aerated structure after baking. (Matsakidou, Blekas, & Paraskevopoulou, 2010).

Baking is a complex heating progress that causes a series of physical, chemical and biochemical changes in the product. The heating induces the dough or cake batter to expand at the beginning, eventually leading to moisture loss at its maximum rate. Finally, the dough or batter is set with a decrease in the moisture loss rate, and the finished products become aerated and light. These mechanisms occur as a function of temperature (Al-Muhtaseb, Hararah, Megahey, McMinn, & Magee, 2010). A typical baking processes produces numerous compounds, for example, acrylamide and the Maillard reaction products (Nursten, 2005). The formation of these contaminants is believed to increase exponentially with baking temperature up to 220 °C. Hypothetically, MCPD esters and GE will be formed through baking processes.

1.2 Objectives

Therefore, this study aimed to evaluate the analysis method (GC-MS/MS and FTIR), formation and mitigation of the formation of 3- and 2-MCPD esters and GE in related baking products and during the baking process. In detail, the research objectives follow.

1. To make comparison assessment between selected ion monitoring (SIM) and multiple reaction monitoring (MRM) mode in the mass spectrometric analysis of MCPD ester and GE.
2. To evaluate the effects of different shortenings in combination with different baking temperatures on the physical qualities, stability of the fat portion and the MCPD esters and GE content a cup cake recipe.
3. To determine the effects of natural and synthetic antioxidant fortification into selected shortenings on the changes in radical intensity, oxidation state, MCPD esters and GE content.
4. To verity a rapid detection method for MCPD esters and GE from gas chromatography (GCMS) and Fourier transform infrared (FTIR) spectra with chemometric analysis.

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