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**MATHEMATICAL MODELING OF RELEASE OF ANTIOXIDANTS
FROM CHITOSAN FILMS**

MISS PHATSORN WASEYAWAN

**A SPECIAL RESEARCH PROJECT SUBMITTED IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR
THE DEGREE OF MASTER OF ENGINEERING (CHEMICAL ENGINEERING)
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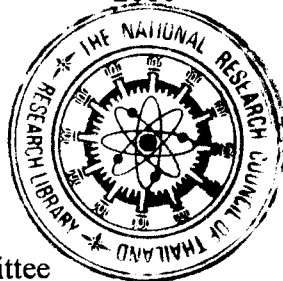
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Mathematical Modeling of Release of Antioxidants from Chitosan Films

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Abstract

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Antioxidants are nowadays added to many types of food packagings, especially packaging films, to enhance their effectiveness in protecting food from an environment. This positive action is possible due to the release of the agents from the film matrix into food to reduce oxidation, thus extending the product shelf life. For effective design of antioxidant-added films, the release characteristics of antioxidants from the films under various conditions need to be known. The aim of this study was to test various simple mathematical models for prediction of the release of antioxidants from edible chitosan films into distilled water at room temperature; chitosan films were prepared via hot air drying, vacuum drying and low-pressure superheated steam drying. The models with different expressions of the effective diffusivity were tested. The model equations were solved numerically using the finite element method via COMSOL Multiphysics™ software (version 3.5). The prediction efficiency of the models was verified by comparing the predicted release kinetics of the antioxidants, in terms of the total phenolics content (TPC), with the experimental data of Mayachiew et al. (2010). It was found that the model assuming the effective diffusivity as a function of the phenolics concentration gave the best agreement with the experimental results.

Keywords: Antioxidant / Chitosan Films / Diffusion / Distilled water / Effective Diffusivity / Mathematical Model

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บทคัดย่อ

ปัจจุบันมีการเติมสารต้านอนุมูลอิสระชนิดต่างๆ ลงในบรรจุภัณฑ์สำหรับอาหาร โดยเฉพาะอย่างยิ่งฟิล์มห่อหุ้มอาหาร เพื่อเพิ่มประสิทธิภาพในการปกป้องอาหารจากสิ่งแวดล้อม ทั้งนี้สารต้านอนุมูลอิสระที่เติมลงไปจะแพร่จากเนื้อฟิล์มไปยังอาหารและช่วยลดการเกิดปฏิกิริยาออกซิเดชันในอาหาร จึงสามารถยืดอายุการเก็บรักษาของอาหารนั้นได้ ในการออกแบบฟิล์มที่มีการเติมสารต้านอนุมูลอิสระอย่างมีประสิทธิภาพนั้นจำเป็นต้องทราบพฤติกรรมการปลดปล่อยของสารต้านอนุมูลอิสระจากฟิล์มภายใต้สภาวะต่างๆ งานวิจัยนี้จึงมีวัตถุประสงค์เพื่อทดสอบแบบจำลองทางคณิตศาสตร์อย่างง่ายสำหรับทำนายคุณลักษณะการปลดปล่อยของสารต้านอนุมูลอิสระจากฟิล์มไคโตซานไปยังน้ำกลั่นที่อุณหภูมิห้อง ซึ่งฟิล์มไคโตซานเตรียมโดยการอบแห้งแบบลมร้อน สุญญากาศ และไอน้ำร้อนขดขึงที่สภาวะความดันต่ำ ทั้งนี้ทำการแก้สมการของแบบจำลองที่ใช้สมการสำหรับทำนายค่าสัมประสิทธิ์การแพร่ยังผลที่แตกต่างกัน โดยระเบียบวิธีไฟไนต์เอลิเมนต์ผ่านโปรแกรมสำเร็จรูป COMSOL Multiphysics™ เวอร์ชัน 3.5 จากนั้นจึงนำผลการจำลองที่ได้มาเปรียบเทียบกับผลการทดลองเพื่อเปรียบเทียบประสิทธิภาพการทำนายของแบบจำลองทางคณิตศาสตร์ต่างๆ ที่ทำการทดสอบ ทั้งนี้ทำการเปรียบเทียบผลการจำลองกับผลการทดลองในแง่ของปริมาณสารฟีนอลิกทั้งหมด (TPC) (Mayachiew et al., 2010) จากผลการเปรียบเทียบพบว่าแบบจำลองที่สมมติให้ค่าสัมประสิทธิ์การแพร่ยังผลเป็นฟังก์ชันของความเข้มข้นของปริมาณสารฟีนอลิกทั้งหมดให้ผลใกล้เคียงกับผลการทดลองมากที่สุด

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LIST OF SYMBOLS

a_1, a_2	=	Constants
c	=	Concentration (mg/g film)
c_a	=	Additive concentration (mg/g film)
c_{TPC}	=	Concentration of phenolics in chitosan film (mg/g dried film)
c_{TPC0}	=	Initial concentration of phenolics (mg/g dried film)
c_w	=	Water concentration (g/g dried film)
c_{w0}	=	Initial concentration of water (g/g dried film)
D	=	Diffusion coefficient (m^2/s)
D_{eff}	=	Effective diffusion coefficient (m^2/s)
j	=	Mass flux ($\text{mg}/\text{m}^2\text{s}^2$)
k	=	Constant
$L(t)$	=	Half of film thickness (μm)
M_t	=	Amount of released solute at time t (mg/g dried film)
M_∞	=	Amount of released solute at equilibrium (mg/g dried film)
n	=	Constant
t	=	Time (s or h)
u	=	Additive volume fraction in swollen region
v	=	Velocity of the glassy/rubbery interface (m/s)
x	=	Distance along the film thickness (μm)

GREEK SYMBOLS

δ	=	Film thickness (μm)
δ_r	=	Thickness of swollen layer (μm)
λ	=	Relaxation time (s)
θ	=	Water diffusion time (s)

ABBREVIATIONS

De	=	Deborah number
MSE	=	Mean square error
R^2	=	Correlation coefficient
S_w	=	Swelling interface number