

# Accepted Manuscript

Phospholipids in chocolate: Structural insights and mechanistic explanations of rheological behavior by coarse-grained molecular dynamics simulations

Moritz Kindlein, Ekaterina Elts, Heiko Briesen



PII: S0260-8774(18)30069-4

DOI: [10.1016/j.jfoodeng.2018.02.014](https://doi.org/10.1016/j.jfoodeng.2018.02.014)

Reference: JFOE 9169

To appear in: *Journal of Food Engineering*

Received Date: 20 November 2017

Revised Date: 13 February 2018

Accepted Date: 16 February 2018

Please cite this article as: Kindlein, M., Elts, E., Briesen, H., Phospholipids in chocolate: Structural insights and mechanistic explanations of rheological behavior by coarse-grained molecular dynamics simulations, *Journal of Food Engineering* (2018), doi: 10.1016/j.jfoodeng.2018.02.014.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Phospholipids in chocolate: structural insights and mechanistic explanations of rheological behavior by coarse-grained molecular dynamics simulations

Moritz Kindlein, Ekaterina Elts, Heiko Briesen

*Technische Universität München, School of Life Sciences Weihenstephan, Process Systems Engineering, Gregor-Mendel-Str. 4, 85354 Freising, Germany*

---

## Abstract

The structural properties of phospholipid layers and micelles at sucrose crystal cocoa butter interfaces were investigated by coarse-grained molecular dynamics simulations to understand the molecular mechanisms and structures vital for the chocolate conching process. Influences of the different hydrophilic head groups phosphatidylcholine, phosphatidylethanolamine, phosphatidylinositol, and phosphatidic acid of lecithin phospholipids as well as influences of the degree of saturation of aliphatic chains were investigated. Phospholipid monolayers at sucrose-cocoa butter interfaces were shown to have similar molar composition as soy lecithin, indicating that all phospholipids adsorb with similar probability. Phospholipids with saturated aliphatic chains have smaller areas per lipid in the monolayer on the sucrose cocoa butter interface than unsaturated phospholipids. It was shown that phospholipids that are not adsorbed in the monolayer assemble in spherical, cylindrical, and wormlike micelles in cocoa butter, depending on the phospholipid concentration. Wormlike micelles were shown to be able to build a hydrophilic network in the cocoa butter medium. This is proposed as an explanation for the increasing yield values at higher lecithin concentrations in chocolate manufacturing which have been reported in several studies. The resulting structures of phospholipids on sucrose surfaces were related to experimental measurements from the literature.

---

*Email address:* [heiko.briesen@mytum.de](mailto:heiko.briesen@mytum.de) (Moritz Kindlein, Ekaterina Elts, Heiko Briesen)

Download English Version:

<https://daneshyari.com/en/article/6664601>

Download Persian Version:

<https://daneshyari.com/article/6664601>

[Daneshyari.com](https://daneshyari.com)