Journal of Food Engineering 119 (2013) 602–610

Contents lists available at SciVerse ScienceDirect

Journal of Food Engineering

journal homepage: www.elsevier.com/locate/jfoodeng

A discrete stochastic model for oil migration in chocolate-coated confectionery

Pieter Van der Weeën [a,*], Nathalie De Clercq [b], Jan M. Baetens [a], Claudia Delbaere [b], Koen Dewettinck [b], Bernard De Baets [a]

[a] KERMIT, Department of Mathematical Modelling, Statistics and Bioinformatics, Ghent University, Coupure links 653, 9000 Ghent, Belgium
[b] FTE, Laboratory of Food Technology and Engineering, Department of Food Safety and Food Quality, Ghent University, Coupure links 653, 9000 Ghent, Belgium

ARTICLE INFO

Article history:
Received 20 February 2013
Received in revised form 21 June 2013
Accepted 24 June 2013
Available online 4 July 2013

Keywords:
Cellular automata
Chocolate
Oil migration
Simulation
Stochastic model

ABSTRACT

Oil migration is an important process in the formation of fat bloom on chocolate-coated confectionery, leading to consumer rejection. However, the exact mechanisms behind this phenomenon are still not completely elucidated, which hampers the development of a mathematical simulation model. In this paper, a model based on a cellular automaton (CA) is proposed and parameterized using experimental data obtained from confectionery model systems. This CA-based model is shown to be able to describe the oil migration in an adequate manner and can therefore be used to calculate an effective diffusion coefficient. Further, the potential of a CA-based approach for the further investigation of the fat bloom mechanisms is demonstrated by means of a case study where capillary rise is incorporated in the CA-based model.

1. Introduction

Belgian pralines, commonly known as Belgian chocolates, were first introduced in 1912 by Jean Neuhaus II, a Belgian chocolatier. They usually contain a hard chocolate coating with a softer, for example (hazel)nut-based, filling. Today, Belgian pralines still have an excellent reputation on the international market. However, the whitish haze formed over time on the surface of chocolate, known as fat bloom, poses a worrisome problem hampering the export of these products (Hartel, 1999). This haze is the result of dispersion of light on small fat crystals that are formed when recrystallization occurs at the surface. Fig. 1 shows a microscopic image (156× magnification) of the surface of a bloomed praline. Fat bloom occurs on all chocolate products, but the presence of a liquid filling accelerates the process as the filling oils are often completely liquid at room temperature and can therefore easily transfer through the chocolate coating to the surface (Lonchampt and Hartel, 2004). Bloomed pralines are harmless and still consumable, but a softening of the chocolate coating, a hardening of the filling, a flattening of the taste and most importantly a rejection of the pralines by the consumers due to the association with inferior and expired products may occur (Khan and Rousseau, 2006). A solution to this problem would therefore be very valuable for this multimillion dollar industry. Unfortunately, the actual mechanisms behind fat bloom remain speculative and a more thorough understanding is necessary to better abate quality deterioration. This knowledge can aid a manufacturer to determine a priori the effect on the rate and amount of fat bloom when changing an ingredient or process. Therefore, there is a need to develop better models that combine mass transfer with the phase behavior for accurately predicting the migration of liquid fat and the occurrence of fat bloom (Aguilera et al., 2004; Ghosh et al., 2002; Loisel et al., 1997).

The phenomenon of fat bloom is presented schematically in Fig. 2. A crucial step in the formation of fat bloom is the migration of liquid fat to the surface. Several hypotheses and mechanisms have been put forward to explain oil migration in chocolate. Originally, the driving force for the migration was believed to be diffusion due to a difference in liquid fat content (Ghosh et al., 2002), but nowadays diffusion is ascribed to a gradient in triacylglycerol (TAG) concentration between the chocolate coating and the filled center (Aguilera et al., 2004). The addition of extra cocoa particles and sugar particles is said to retard the oil migration rate, because they are impenetrable to oil (Ghosh et al., 2002). However, a recent study has shown that cocoa particles disrupt the formation of the cocoa butter (CB) crystal network such that the resulting crystal network is less dense and more permeable to oil (Motwani et al., 2011). Besides diffusion, capillary forces may play a significant role and have therefore been proposed as an alternate mechanism of oil migration (Aguilera et al., 2004; Lonchampt and Hartel, 2004).

Another hypothesis for oil migration states that the increase in volume when cocoa butter melts forces liquid fat to the surface

* Corresponding author. Tel.: +32 92645931; fax: +32 92646220.
E-mail address: pieter.vanderweeen@ugent.be (P. Van der Weeën).

0260-8774/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jfoodeng.2013.06.031

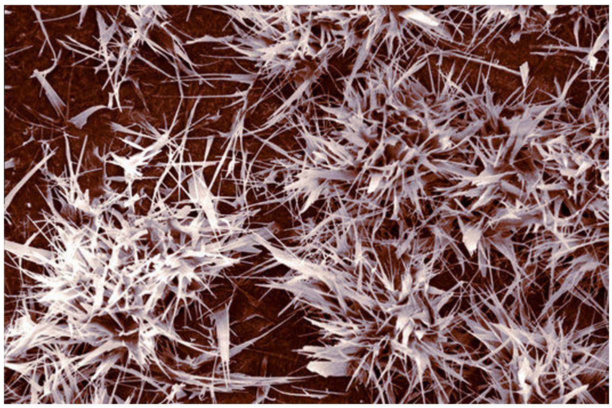

Fig. 1. Microscopic image of the surface of a fat bloomed praline (156× magnification).

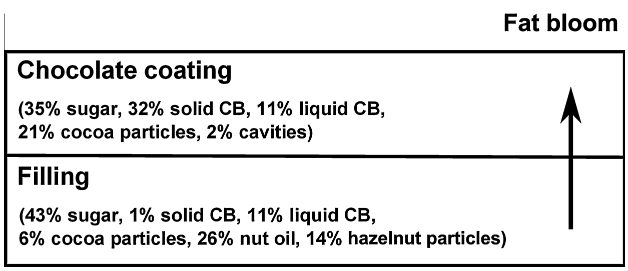

Fig. 2. Schematic representation of fat bloom in chocolate confectionery, with indication of the composition of the different layers in volume percentages.

through pores and micro-fractures formed during crystallization (Kleinert, 1961). Several other theories focus on the thermal stability of the different polymorphic forms of cocoa butter as the cause of fat bloom (Aguilera et al., 2004), but although bloom formation is accompanied by a polymorphic transition of cocoa butter, it is by itself not sufficient to always cause visual fat bloom (Lonchampt and Hartel, 2004). In literature, there is neither a consensus on which mechanisms actually play a role nor on their relative importance, but most papers focus on the diffusion of triacylglycerols and the capillary rise or a combination of both.

In this paper, the CA paradigm, used to construct a stochastic CA-based model, is discussed. Further, the experimental setup and data acquisition, necessary to parameterize the model, are explained. Finally, the potential of such a CA-based model is demonstrated by means of the addition of capillaries to the basic model.

2. Cellular automata

Cellular automata appear for the first time in literature in the first half of the 20th century (von Neumann, 1951) and are mathematical constructs in which the time, space and state domain are discrete as opposed to partial differential equations (PDEs) in which these three domains are continuous (Berec, 2002; Wolfram, 1983). However, a CA-based model can be seen as an alternative to a PDE-based model, because any physical system satisfying PDEs may be approximated by a CA-based model upon introducing finite differences and discrete state variables (Matsukidaira and Nishinari, 2003; Reichenbach et al., 2008). The ability of a CA to generate a rich spectrum of sometimes very complex spatio-temporal patterns from relatively simple underlying transition functions has stimulated the development of various CA-based models to describe tumor growth (Mallet and De Pillis, 2006; Preziosi, 2003), biofilm dynamics (Picioreanu et al., 1998), protein chemistry (Vasilkoski and Weaver, 2000), chemical reaction kinetics (Van der Weeën et al., 2011) and many other phenomena (Ilachinski, 2001; Schiff, 2008; Wolfram, 1983). Many of these models show good performance and are successful in describing nature in a mathematical way (Kier et al., 2005). The use of stochastic CA-based models, which will be employed in this paper, to describe physico-chemical processes is already reported in literature (Chopard and Droz, 1998; Kier et al., 2005).

2.1. Choice of an appropriate model

Many authors have described the fat bloom phenomenon, the influence of different process parameters on the degree and instant of appearance of visual fat bloom and possible causes for this blooming (Ghosh et al., 2002; Khan and Rousseau, 2006; Loisel et al., 1997; Motwani et al., 2011). They often support their theories through a series of calculations based on the governing physical laws that are often expressed as (P)DEs (Aguilera et al., 2004; Ziegler et al., 2004). Continuous models, making use of PDEs, are established mathematical constructs, also in the field of food engineering, that are often transparent in terms of how a change in their parameters affects the simulation results and are therefore relatively understandable (Hanspal et al., 2009; Lee and Koon, 2009; Weimar et al., 1992). However, establishing and solving a system of PDEs for a specific process still remains tedious, while the numerical approximation techniques unavoidably give rise to approximation errors and stability problems (El Yacoubi and El Jai, 2002; Toffoli, 1984). Moreover, PDE-based modeling constitutes a roundabout approach if one considers that it first involves the derivation of a set of continuous equations from discrete mass balances after which these equations have to be discretized again as it is for most practical problems impossible to retrieve an analytic solution (Toffoli, 1984).

PDE-based models for oil migration and fat bloom have been developed, but choosing the appropriate governing equations that mimic these processes is nontrivial as the exact mechanism behind both is not known (cfr. Section 1). This makes that the solution of the governing PDEs, even after simplification, does not always lead to physically meaningful results (Romero et al., 2009). Furthermore, the stochasticity of the process at stake can be of great importance, but difficult to capture with traditional kinetic models (di Caprio et al., 2011).

In light of the aforementioned problems and given the fact that only few authors have attempted to develop an elucidatory or descriptive model for fat bloom, the search for a full-fledged mathematical model accurately describing fat bloom is ongoing. Therefore, a CA-based model is proposed in this paper. CAs are still not as popular as PDEs, although an increasing number of researchers is employing them, also in the field of food engineering (Martins and Lopes, 2007). Moreover, it is reported that CAs have great potential to simulate natural phenomena when there is no other mathematical model available (Bandman, 2002, 2008), because the often intractable dynamics are translated into a transition function that mirrors intuition and is easy to compute (Ilachinski, 2001; Schiff, 2008). Once a phenomenon's underlying processes are broken down into discrete activities, it can be represented with a CA-based model, as such providing new discrete dynamical approaches to microscopic physics (Schiff, 2008). In fact, some CA-based models produce results nearly identical to laboratory experiments (Lejeune et al., 1999). In addition, CAs can deal with heterogeneity (Baetens and De Baets, 2012; Berjak and Hearne, 2002; Kuntz et al., 1997), which in case of oil migration in chocolate-coated confectionery can yield a way to study the effect of capillarity. The number, position and size of capillaries in the chocolate coating can be varied without having to deal with the implementation of boundary conditions.