SciVerse ScienceDirect

Procedia Food Science 1 (2011) 340 – 346

Procedia Food Science

11th International Congress on Engineering and Food (ICEF11)

Modelling crystal polymorphisms in chocolate processing

Serafim Bakalis* , Benjamin J.D. Le Révérend, Nurul Z. Rois Anwar, Peter J. Fryer

School of Chemical Engineering, University of Birmingham, Edgbaston, Birmingham,B15 2TT (s.bakalis@bham.ac.uk)

Abstract

Efforts have been devoted over the last decades towards modelling phase change kinetics of fats in chocolate. The fats in chocolate have a number of polymorphic forms and manufacturers must deliver a product with the right polymorph to the consumer. In this work a model was developed that contains only two polymorphs rather than the six polymorphs that can be identified using Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD). This simplification allowed the phase change kinetics to be estimated from a set of DSC experiments. The phase change reactions were coupled with heat transfer and used to successfully predict the temperature profiles and the concentration of polymorphs (within 10%). These quantities determine among others contraction and cohesion, which are essential to demoulding and cleaning processes. Indeed, deposits left on the mould surface leads to undesirable product surface and an increase of cleaning costs. During the rapid cooling step (similar to the FrozenCone process), only a thin layer (to maintain the prescribed shape) of the shell is partially crystallised (typically 20% of the thickness) with unstable crystals (typically 10%) due to the high cooling rates. The model was then used to develop of a rapid cooling process allowing the estimation of the processing time required for the rapid cooling step depending on the thickness of the shell and the temperature of the plunger.

Keywords Chocolate; polymorphism; rapid cooling; phase change; mathematical modelling

1. Introduction

Traditional chocolate processing typically involves a slow cooling (<2°C/min) after the tempering stage [1]. During the tempering stage a series of cooling and heating steps, which selects fat crystals of form βV. These crystals, as opposed to the β' crystals, have a melting point close to body temperature and are stable at room temperature [2]. This presents an opportunity to control product structure by controlling

* Serafim Bakalis. Tel.: (+44) (0)121 414 5383; fax: (44) 121 4145324.
E-mail address: S.Bakalis@bham.ac.uk

2211 601X
doi:10.1016/j.profoo.2011.09.053

temperature histories during processing [3,4] – the design of successful healthy products will depend on the delivery of taste and flavour indistinguishable from the original. Novel structures could be of value in the creature of foods that have healthier properties.

If the tempering process is successful, the microstructure of the cocoa butter in chocolate is strongly dependent on the cooling rate applied to the chocolate during processing. Recent progress in chocolate manufacturing has led to rapid cooling processes (≈100 ^{o}C/min) at the interface between the chocolate and the plunger), and these fast cooling rates do not necessarily ensure that only the βV form of cocoa butter will be crystallised. The crystallisation of lower stability polymorphs is a problem for the manufacturers since it can lead to an acceleration of the blooming problem (during the polymorphous transition), making the chocolate unacceptable for the consumer.

The modelling of chocolate cooling has been extensively investigated [5-8] but to the best of our knowledge there is no model coupling the heat transfer occurring in the product during solidification and the crystallization kinetics of the fat crystal network. The challenges presented for such a model are the polymorphism of cocoa butter and the lack of temperature dependent data for the phase change kinetics of cocoa butter.

The adhesive force (between the chocolate and the mould surface) and the cohesive force (between elements of the chocolate itself) that affect both demoulding and the subsequent cleaning process are strongly dependent on the structure of the product. In the case of chocolate, this is related to the crystal structure obtained during processing and the interaction between the chocolate and the mould surface. The adhesive or/and cohesive failure will determine the ease of demoulding stage and eventually influence the product quality characteristics.

This paper presents a simplified model of chocolate cooling, validated using XRD data and a range of temperature profiles [9-11]. The model was also extended to the FrozenCone® process [12] using commercial finite element software.

2. Materials and Method

2.1 Mathematical model

The model used to describe the cocoa butter phase change kinetics and polymorphism is based on the hypothesis that the polymorphs can be split into two main categories: the *unstable* and the *stable* crystals. This hypothesis is supported by XRD and DSC data. The unstable crystals are α and β' while the stable crystals are β crystals. *Unstable* crystals have a very strong *d*-spacing around 4.3Å while *stable* crystals have very strong *d*-spacings at 4.6Å [13,14]

The model therefore considers six different reactions, each of them associated with a reaction rate dependent on temperature (step change around the phase change temperature). The heat transfer equation (1) was solved together with three differential equations for mass balance on the three phases of the system (2).

$$\rho.Cp.\frac{\partial T}{\partial t} = \nabla.(k.\nabla T) + Q_{source} \qquad (1)$$

where ρ is the density of the chocolate, Cp its specific heat, k its thermal conductivity and Q_{source} the heat source associated with the phase changes of cocoa butter.

The phase changes of cocoa butter were solved according to the system of PDEs defined in (2). The system was simplified to only two polymorphs as explained in the introduction.