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Identification of the significant factors in food quality using global sensitivity analysis and the accept-and-reject algorithm. Part III: Application to the apple cold chain

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ABSTRACT

The aim of this manuscript is to apply the methodology proposed in an accompanying part I describing the different sources of variability in the apple cold chain allowing the identification of significant factors on the evolution of apple quality. The methodology uses a deterministic model to predict the evolution of quality (firmness, colour) and stochastic models to account for the variability of product time–temperature history, biological properties and initial quality. Hereto, a dedicated field test to obtain a realistic set of time–temperature data for the long term controlled atmosphere (CA) storage of apple was conducted. The apple cold chain under consideration in this study comprises the following links: pre-cooling, CA storage, non-refrigerated transport and wholesale. Then, the simulation results, using kinetic models for describing the evolution of firmness and colour as influenced by the time–temperature profiles, and following the method presented in part I (global sensitivity analysis and an accept-and-reject algorithm) are analysed. Our research indicated that the product time temperature profile along the cold chain was the most influencing factor on the final apple quality. A refined analysis by the accept-and-reject algorithm revealed the impact of CA storage and pre-cooling.

1. Introduction

Apple skin background colour and firmness are very important quality aspect for consumers who prefer products with a uniform quality (Gwanpua et al., 2013). However, the management of uniform quality is a tedious task for postharvest handlers because of many sources of variability, such as inherent biological variation and fluctuations in time temperature profile of fruit along the cold chain. The biological variation is a consequence of several factors. Apples harvested at different dates will ripen differently (Gwanpua et al., 2013). Fruit-to-fruit variation is observed for apples picked in the same batch, and this is resulting from differences in shading, orientation of the fruit on the tree, and types or levels of fungicides (Kingston, 2010). Over the last decades, models including biological variance to explain the propagation of biological variation in fruit were widely developed (Hertog et al., 2004, 2007; Mziou et al., 2009). The quality evolution of fruit such as firmness and colour depends on the gas composition in air, but also on time and storage temperature. Along the cold chain, apples can be stored at different temperature during different periods. The temperature and its variability can be different according to the equipment. Several field studies were carried out on refrigerated products in the cold chain (Laguerre et al., 2002; Morelli and Derens, 2009; Rediers et al., 2009; Derens-Bertheau et al., 2014). Such data have already been combined with quality model evolution to identify the impact of the time temperature profile on the final quality, mostly in case-studies related with microbiological safety modelling (Afchain et al., 2005; Pouillot et al., 2007;

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Nomenclature

$[C_2H_4]$	internal ethylene concentration (mmol m^{-3})
$[C_2H_4]_{ref}$	reference ethylene concentration (mmol m^{-3})
$[Chl]$	chlorophyll content of the skin (nmol cm^{-2})
$[E_{Chl}]$	chlorophyllase concentration (mmol m^{-3})
Col	background skin colour of apple (a^*)
Col_c	fixed part of the background skin colour (a^*)
$E_{a,i}$	activation energy for reactions (J mol^{-1})
$[E_{pect}]$	normalized concentration of the pectin degrading enzyme
F	firmness (N)
F_0	initial firmness (N)
F_c	part of firmness not affected by the enzymatic breakdown (N)
f_{clim}	transition from preclimacteric stage ($f_{clim} = 0$) to climacteric stage ($f_{clim} = 1$)
$k_{C_2H_4}$	rate of diffusion of ethylene from the apple to its surrounding (d^{-1})
k_{Chl}	rate constant for chlorophyll breakdown (mmol m^{-3} d^{-1})
$k_{Chl,\ ref}$	reference rate constant for chlorophyll breakdown (mmol m^{-3} d^{-1})
$k_{E_{Chl}}$	rate constant for synthesis of *Chlase* (m^3 $mmol^{-1}$ d^{-1})
$k_{E_{Chl},\ deg}$	rate constant for turnover of *Chlase* (d^{-1})
k_{clim}	transition rate between preclimateric stage to climacteric stage
$k_{E_{pect}}$	rate constant for the synthesis of E_{pect} (m^3 $mmol^{-1}$ d^{-1})
$k_{E_{pect},deg}$	rate constant for the turnover of E_{pect} (d^{-1})
k_i	rate constant
$k_{i,\ ref}$	reference value of rate constant k_i
K_{m,O_2,C_2H_4}	Michaelis-Menten constants for ethylene production (kPa)
K_{mu,CO_2,C_2H_4}	Michaelis-Menten constants for uncompetitive inhibition of ethylene production by carbon dioxide (kPa)
k_{pect}	rate constant for pectin breakdown (mmol m^{-3} d^{-1})
$k_{pect,\ ref}$	reference rate constant for pectin breakdown (mmol m^{-3} d^{-1})
$[P]$	amount of unhydrolyzed pectin (mmol m^{-3})
p_{O_2}	external partial pressure of oxygen (kPa)
p_{CO_2}	external partial pressure of carbon dioxide (kPa)
R	universal gas constant (J mol^{-1} K^{-1})
T	product temperature (°C)
T_{ref}	reference temperature (°C)
t_{rs}	residence time (d)
V_{m,C_2H_4}	maximum rate of ethylene production (mmol m^{-3} d^{-1})
$V_{m,C_2H_4,\ ref}$	reference maximum rate of ethylene production (mmol m^{-3} d^{-1})
γ	correlation factor between unhydrolyzed pectin and firmness (N $mmol^{-1}$ m^3)

Couvert et al., 2010; Ellouze et al., 2010; Koutsoumanis et al., 2010; De Cesare et al., 2013).

Among several approaches to account for the variability, the Monte Carlo method is widely used for its robustness and its ease of implementation. In food engineering, this method combines stochastic models to describe the variability of biological parameters (De Ketelaere et al., 2004; Hertog et al., 2009; Gwanpua et al., 2013) or time temperature profiles (Hoang et al., 2012; Duret et al., 2013) and deterministic models to describe quality evolution (microbial growth, firmness, colour…). Its main drawback is the calculation time due to the needs of a large number of repetitive simulations. However, it is not limited neither by the number of the stochastic variables involved nor by the complexity of the model describing the studied process. It was applied in postharvest science by Hertog et al. (2009) to model variability in the Hue colour in tomato and by De Ketelaere et al. (2004) to predict tomato shelf-life.

Part I of this study describes the methodology to account for the different sources of variability and the methods used to identify properly the significant factors on final food quality (Duret et al., 2014) for use in the FRISBEE tool (Gwanpua et al. (in press, 2014)), a software for assessing refrigeration technologies, developed within the framework of the European Union FP7 project, FRISBEE (Food Refrigeration Innovations for Safety, consumers' Benefit, Environmental impact and Energy optimization along the cold chain in Europe). The aim of the present manuscript is to apply the methodology to study the evolution of both the firmness and the colour of apples from harvest until wholesale.

2. Materials and methods

2.1. Overview of the methodology

The modelling methodology was presented in the part I (Duret et al., 2014). This part proposed a methodology combining a deterministic model to calculate the product quality evolution and stochastic models for considering difference sources of variability in the cold chain (product temperature in equipment, residence time, initial quality, biological variability of products). Then, a methodology based on global sensitivity analysis (SA) and accept-and-reject algorithm (AR) was proposed to identify the most influencing factors on the product final quality. The global methodology is presented in Fig. 1. Section 1 presents the model inputs, Section 2 the models used, and Section 3 the methods used to identify the significant factors on apple final quality. The quality evolution is predicted from pre-cooling after harvest to the wholesale.

2.2. Modelling the product time temperature history

The time temperature history of the product throughout the cold chain was modelled using a combination of data (Table 1). To obtain a realistic set of time temperature data for the long term CA storage of apple a dedicated field test was conducted by the Flanders Centre of Postharvest Technology (Belgium). The test was in cooperation with three Belgian apple growers and measured the time temperature profile from harvest up to and including the long term CA storage. The test started in October 2012 and ran for as long as the grower kept his apples in CA storage which was, depending on the apple grower, November 2012 to April 2013. Data for the subsequent steps of the cold chain were gathered from the cold chain database which was developed within the framework of the FRISBEE project. It concerned data of tomatoes and bell peppers, having the same distribution chain as apples: after being bought at the auction, they are transported to the wholesale and subsequently to retail. Temperature and residence time profiles were described by a normal and exponential distribution, respectively.

In this study, the following steps in the apple cold chain were included: pre-cooling after harvest, CA storage, transport and