Postharvest Biology and Technology 136 (2018) 31–41

Contents lists available at ScienceDirect

Postharvest Biology and Technology

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

Model based leak correction of real-time RQ measurement for dynamic controlled atmosphere storage

N. Bessemans[a], P. Verboven[a], B.E. Verlinden[b], B.M. Nicolaï[a,b,*]

[a] KU Leuven, BIOSYST/MeBioS, Willem de Croylaan 42, 3001 Heverlee, Belgium
[b] Flanders Centre of Postharvest Technology, Willem de Croylaan 42, 3001 Heverlee, Belgium

ARTICLE INFO

Keywords:
Respiration
Dynamic controlled atmosphere
Air tightness
Model
Gas flow
Apple fruit

ABSTRACT

A method was developed to correct real-time measurements of the respiratory quotient (RQ) of pome fruit for gas leakage of a cool room. The method is based on a general leakage model that was simplified by performing sensitivity analysis of the contribution of the pressure driven and concentration driven gas transport terms. The analysis showed that pressure driven leakage was dominant over diffusive leakage. The methodology was validated successfully using an empty storage container at 0.4 kPa O_2 and 1.3 kPa CO_2. A sensitivity analysis using virtual storage experiments showed that the error of the RQ estimates with leak correction was 0%, while without leak correction they increased to above 700%. Finally, the validated model was successfully implemented in an automated RQ-DCA control system using 'Braeburn' apple fruit (*Malus* × *domestica* 'Braeburn' 2*x*). RQ estimates without leakage correction were heavily biased when leakage of atmospheric air into the storage container occurred and would lead to erroneous control of the storage atmosphere composition. With the developed leakage correction, RQ measurements were found to be accurate during decreasing as well as increasing atmospheric air pressure.

1. Introduction

Controlled atmosphere (CA) storage systems are widely used to preserve quality of apple fruit. During CA storage, fruit are exposed to a decreased O_2 partial pressure, an increased CO_2 partial pressure and a low temperature (Dilley, 2010; Ho et al., 2013). CA storage is intended to slow down respiration and other quality degradation processes that are associated with respiration (Saltveit, 2003; Verboven et al., 2006; Both et al., 2017). Optimal storage conditions are usually determined empirically as to deliver good quality after storage (Peppelenbos, 2003; Wright et al., 2012; Nock and Watkins, 2013). To avoid off-flavor and storage disorders, these optimal storage conditions usually maintain a safety margin relative to the anaerobic compensation point (ACP) − the O_2 concentration at which CO_2 production is minimal. The anaerobic compensation point is the O_2 concentration below which the metabolism of the stored fruit changes from aerobic respiration to fermentation as main energy source, leading to off-flavor and storage disorders (Kader, 1989; Fonseca et al., 2002; Geigenberger, 2003; Franck et al., 2007; Thewes et al., 2015). At O_2 concentrations above the ACP respiration rapidly increases with O_2 concentration, leading to increased quality loss during storage (Burg and Burg, 1965). The safe margin maintained regarding the ACP with conventional CA storage provides an opportunity to improve post-storage fruit quality by further reducing in-cool room O_2 levels and minimizing fruit respiration by storing the fruit as close as possible to − and ideally at the ACP. An additional benefit of storing fruit at low O_2 concentrations, is the reduction of O_2 related storage disorders like superficial scald, which otherwise need to be prevented in a chemical way by treatment with anti-scald agents like diphenylamine (DPA) and ethoxyquin or the ethylene blocker 1-methylcyclopropene (1-MCP) (DeEll et al., 1996; Blankenship and Dole, 2003; Watkins, 2008; Lurie and Watkins, 2012).

State of the art storage technologies like dynamic controlled atmosphere (DCA) storage, search for the lower oxygen limit (LOL) of the stored produce − which is the lowest O_2 concentration at which the fruit can be stored without developing off-flavor and storage disorders (Wollin et al., 1985; Zanella, 2003). Thereto, in-cool room O_2 concentrations are gradually decreased during storage until low O_2 stress is detected based on real-time measurement of a bio-response of the stored fruit to low O_2 stress (Wolfe et al., 1993). Subsequently, the O_2 concentration is increased again until relief of low O_2 stress, ensuring the produce is being stored at the lowest O_2 concentration possible, and thereby minimizing quality loss (Veltman et al., 2003; Gasser et al., 2008; Wright et al., 2012).

In the past, the most prominent DCA technologies were based on

---

[*] Corresponding author at: KU Leuven, BIOSYST/MeBioS, Willem de Croylaan 42, 3001 Heverlee, Belgium.
E-mail address: bart.nicolai@kuleuven.be (B.M. Nicolaï).

http://dx.doi.org/10.1016/j.postharvbio.2017.09.011
Received 4 July 2017; Received in revised form 29 September 2017; Accepted 29 September 2017

Nomenclature

A	Leakage area of the storage facility [m^2]
D_i	Diffusivity of gas component i in air at atmospheric air pressure and 274.15 K where i may be O_2 and CO_2 [m^2 s^{-1}]
δ	Thickness of storage facility wall [m]
Δt	Time interval delta t [s]
$H(z) = 0 \quad z < 0$ $= 1 \quad z \geq 0$	Heaviside function of z [−]
k	Leakage constant of the storage facility [mol s^{-1} Pa^{-1}]
L	Length of the joins of the storage facility [m]
m	Mass of the stored produce inside the storage facility [kg]
n_i	Number of moles of gas component i inside the storage facility where i may be O_2, CO_2 and N_2 [mol]
p_i	Partial pressure of gas component i in the storage room where i may be O_2, CO_2 and N_2 [Pa]
$p_{i,a}$	Partial pressure of gas component i in the atmosphere where i may be O_2, CO_2 and N_2 [Pa]
P	Total pressure inside the storage facility [Pa]
P_a	Atmospheric air pressure [Pa]
q_i	Flow rate of gas component i due to leakage where i may be O_2, CO_2 and N_2 [mol s^{-1}]
r_{O_2}	O_2 consumption rate by fruit respiration [mol s^{-1} kg^{-1}]
r_{CO_2}	CO_2 production rate by fruit respiration [mol s^{-1} kg^{-1}]
R	Universal gas constant [J mol^{-1} K^{-1}]
R_{O_2}	Measured O_2 consumption rate by fruit respiration [mol s^{-1} kg]
R_{CO_2}	O_2 consumption rate by fruit respiration [mol s^{-1} kg]
RQ	Instantaneous value of the respiratory quotient [−]
RQ_0	RQ estimate without leak correction [−]
RQ_{ox}	RQ at aerobic conditions [−]
$\overline{RQ}$	Mean value of the respiratory quotient [−]
T	Temperature [K]
t	Time [s]
t_i	[s]
t_f	Time of the end of time interval Δt
τ_{diff}	time constant of the diffusion driven leakage process [s]
τ_{pres}	Time constant of the pressure driven leakage process [s]
V	Free volume inside the storage facility [m^3]
V_{stor}	Total volume of the facility [m^3]
V_{m,O_2}	Maximal O_2 consumption rate [mol m^{-3} s^{-1}]
V_{m,f,CO_2}	Maximal fermentative CO_2 production rate [mol m^{-3} s^{-1}]
K_{m,O_2}	Michaelis-Menten constant for O_2 consumption [kPa]
K_{mn,CO_2}	Michaelis-Menten constant of non-competitive CO_2 inhibition of the O2 consumption rate [kPa]
K_{m,f,O_2}	Michaelis-Menten constant of O_2 inhibition on fermentative CO_2 production [kPa]
x_i	Gas fraction of component i in the storage room where i may be O_2, CO_2 and N_2 [−]
$x_{i,a}$	Gas fraction of component i in the atmosphere where i may be O_2, CO_2 and N_2 [−]

chlorophyll measurements (DCA-CF) and DCA based on measurements of the ethanol content headspace of a small box of sample fruit which is placed inside the cool room (DCS) (Schouten et al., 1997; Prange et al., 2002). More recently, a novel type of DCA storage based on measurements of the respiratory quotient (RQ) of the stored fruit (RQ-DCA) was developed (Delele et al., 2015; Bessemans et al., 2016). The RQ is defined as the ratio of the CO_2 production rate and the O_2 consumption rate of the stored produce (Gran and Beaudry, 1993; Jozwiak and Blanpied, 1993). When aerobic respiration is the main energy source, RQ was found to have a value of about 0.91, 0.91 and 0.90 for 'Jonagold', 'Braeburn' and 'Kanzi' apple fruit respectively (Hertog et al., 2001; Ho et al., 2013). However, when the O_2 concentration approaches zero the fruit metabolism shifts from aerobic respiration to fermentation, resulting in a steep increase in RQ. This increase is therefore a good measure for low O_2 stress (Gran and Beaudry, 1993; Jozwiak and Blanpied, 1993; Yearsley et al., 1997, 1996). RQ-DCA uses real-time estimates of the RQ of the stored fruit in the cool room to alter the CA setpoints continuously throughout the storage season based on measured changes of gas concentrations (Bessemans et al., 2015, 2016; Both et al., 2017, Thewes et al., 2017). Measured changes in CA composition of the cool room atmosphere are mainly caused by consumption of O_2 and production of CO_2 by fruit respiration (Hertog et al., 1998). However, leakiness of the cool room may allow small amounts of atmospheric air to leak inside and vice versa, altering the gas partial pressures of the cool room. Cool room walls may be assumed to be perfectly gastight, but leakage might occur in the seals and seams of the room due to the surface roughness of the materials used (Persson and Yang, 2008). Depending on the surface roughness, elastoplastic properties of the seals and contact pressure, small areas may remain where the seals are not perfectly in contact with the walls (Persson, 2001; Okada et al., 2008). This might result in small percolation channels allowing gas flow between the cool room and environment (Bottiglione et al., 2016; Bottiglione et al., 2009; Zhang et al., 2017).

The importance of leakage modelling and its dependence on seal material properties such as surface roughness in cool rooms has been identified (Nahor et al., 2005). Recently, we have shown that obtaining accurate estimates of RQ at low O_2 partial pressures is difficult when the rate of leakage of respiratory gasses reaches the same order of magnitude as the respiration rate of the stored fruit (Bessemans et al., 2016). This leads to biased RQ calculations, while too high leakage rates make it also impossible to reach the desired low O_2 concentrations.

In this work, a leakage model of postharvest storage facilities was developed to compensate in real-time for leakiness in estimates of RQ of fruit under dynamic controlled atmosphere conditions. The method was validated using an empty storage container experiment. The model was implemented in an automated RQ-DCA control system and successfully used in an experiment to compare estimates of RQ with and without leakage correction simultaneously for a batch of 'Braeburn' apple fruit (*Malus* × *domestica*, 'Braeburn' 2*x*).

2. Materials and methods

2.1. Storage container

Experiments in this work were conducted in a storage container which was placed in a cool room at 1 °C. The container (0.715 m × 0.515 m × 0.965 m) was made of rigid polypropylene (thickness 1 cm) and consisted of a bottom and top lid with an airlock for gastight sealing. It was connected to an in-house built measuring unit that contained a closed measurement circuit with a pump for continuously circulating the storage atmosphere to a measurement chamber and back to the storage container. The measurement chamber contained a galvanic cell type O_2 sensor (Figaro KE50, Figaro USA), a non-dispersive infrared (NDIR) type CO_2 sensor (GE Telaire T6615-50KF 50000 ppm, TELAIRE, USA) and a digital pressure sensor (MEAS MS5611-01BA03, MEAS, Switzerland). Oxygen and CO_2 sensors were calibrated using two different gas mixtures (Air Products N.V., Belgium) of 0 kPa O_2 and 0 kPa CO_2 and 5 kPa O_2 and 5 kPa CO_2. A photograph and schematic representation of the air lock and the storage container