Mathematical Modelling of Modified Atmosphere Packaging Systems for Apples

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Ingeborg Merts
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ABSTRACT

ENZA New Zealand (International) is considering the use of modified atmosphere packaging (MAP) as an adjunct to cool storage for cartons of apples. The objectives of this study were to measure modified atmosphere development in apple cartons and to develop a mathematical model that could be used as a tool for package design and optimization.

Storage trials were carried out with film-lined cartons of 'Braeburn', 'Royal Gala', and 'Granny Smith' apples. Measured package O_2 and CO_2 concentrations showed excellent reproducibility for cartons with heat-sealed liners. Liners closed by folding produced less modified and less consistent package atmospheres, especially for thicker films (40 µm versus 25 µm). Macroscopic holes in the liners resulted in almost total loss of atmosphere modification, whereas microscopic holes resulted in smaller changes apparent for O_2 concentrations only. A high incidence of film damage could quickly erode any potential fruit quality benefits imparted by the liners.

Packing of warm rather than pre-cooled fruit resulted in much faster rates of atmosphere modification, without the development of unduly low O_2 or high CO_2 concentrations. The detrimental quality effects of slower cooling rates for film-lined cartons may outweigh any benefits of more rapid modified atmosphere development. Short-term exposures (less than 24 hours) to 20°C resulted in relatively short-lived and non-critical disturbances to package atmospheres. Periods of more than 3 days at 20°C led to a significant risk of anaerobic conditions or harmful CO_2 levels forming within the fruit, especially within the 40 µm liners. Folding rather than heat-sealing of liners did not reduce this risk.

The MAP model simulated fruit respiration as a function of temperature and fruit O_2 and CO_2 concentrations; O_2, CO_2, N_2, and water vapour exchange between the fruit, package, and external atmospheres; condensation of moisture within the package; and moisture sorption by paper-based packaging materials. Gas concentrations and temperature throughout (i) the fruit and (ii) the package atmosphere were each assumed to be uniform with position. The model can be applied to a wide range of packages under variable-temperature storage regimes. The model closely predicted observed trends in experimental data collected during the MA storage trials, but tended to under-predict CO_2 concentrations and performed less well under conditions of extremely modified atmospheres. Sensitivity analyses showed that this lack of fit was not greater than that which could be explained by uncertainties in respiration and permeability data. It is recommended that future work be aimed at resolving the worst of these uncertainties before a significant amount of effort is directed towards further model development.

The MAP model was considered sufficiently accurate for it to be usefully applied to the design and optimization of MAP systems.

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ERRATA

p. x Sub-sections of section 8.2.1 should be numbered 8.2.1.1, 8.2.1.2, and 8.2.1.3.

p. 13 Second-to-last line of second paragraph. 'Late harvested fruit were used in the trail...' should read 'Late harvested fruit were used in the trial...'.

p. 33 Eq. 2.7. The symbol RQ_m should be RQ (as listed in the definition of symbols on p. 34).

p. 37 Definition of symbols for Eq. 2.12. Units of $[i]_{ext}$ and $[i]_{int}$ should read ($m^3 \cdot m^{-3}$).

p. 96 Eq. 6.14 should read

$$\frac{d\left(\varepsilon V_n C_{O_2,f}\right)}{dt} = k_{O_2} A_n \left(C_{O_2,p} - C_{O_2,f}\right) - vM_n$$

p. 114 Eq. 6.85 should read

$$\frac{d\theta}{dt} = -\alpha\left(\theta - \theta_e\right)$$

p. 121 Throughout Chapter 7, the symbol 'ε' represents the local error tolerance bound for the numerical solution method. Throughout the rest of the thesis 'ε' represents the porosity of the fruit flesh ($m^3 \cdot m^{-3}$).

p. 151 Section 8.2.2.1 should be numbered 8.2.1.1.

p. 155 Section 8.2.2.2 should be numbered 8.2.1.2.

p. 158 Section 8.2.2.3 should be numbered 8.2.1.3.

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NOMENCLATURE

This section lists the nomenclature used in the mathematical formulation of the MAP model (Chapter 6). Miscellaneous symbols used locally in Chapters 2, 4, 7, and 8 are defined in the text as necessary.

a	empirical parameter of the fruit surface area-volume correlation (Eq. 6.17)
A_{film}	total surface area for gas permeation through the packaging film (m^2)
A_{fruit}	total fruit surface area (m^2)
A_{holes}	total area of holes in the packaging film (m^2)
A_n	individual fruit surface area (m^2)
A_{pack}	average heat transfer area of the packaging materials (m^2)
A_{tray}	effective tray surface area for moisture sorption ($m^2 \cdot tray^{-1}$)
a_w	fruit water activity
$a_{w,\ tray}$	tray water activity
b	empirical parameter of the fruit surface area-volume correlation (Eq. 6.17)
Bi	Biot number for heat transfer
Bi'	Biot number for mass transfer
c_{pa}	specific heat capacity of dry air ($J \cdot kg^{-1} \cdot K^{-1}$)
c_{pf}	specific heat capacity of the fruit flesh ($J \cdot kg^{-1} \cdot K^{-1}$)
c_{pt}	specific heat capacity of the dry trays ($J \cdot kg^{-1} \cdot K^{-1}$)
c_{pv}	specific heat capacity of water vapour ($J \cdot kg^{-1} \cdot K^{-1}$)
c_{pw}	specific heat capacity of liquid water ($J \cdot kg^{-1} \cdot K^{-1}$)
C	parameter of the GAB isotherm model (Eq. 2.22)
$C_{CO_2,\ e}$	CO_2 concentration in the store atmosphere ($kg\ CO_2 \cdot m^{-3}$)
$C_{CO_2,\ p}$	CO_2 concentration in the package atmosphere ($kg\ CO_2 \cdot m^{-3}$)
$C_{CO_2,\ f}$	CO_2 concentration in the fruit internal atmosphere ($kg\ CO_2 \cdot m^{-3}$)
$C_{H_2O,\ p}$	concentration of water vapour in the package atmosphere ($kg\ H_2O \cdot m^{-3}$)
$C_{H_2O,\ e}$	concentration of water vapour in the store atmosphere ($kg\ H_2O \cdot m^{-3}$)
C_i	mass concentration of gas species i ($kg \cdot m^{-3}$)
$C_{i,e}$	ambient concentration of gas species i ($kg \cdot m^{-3}$)
$C_{i,p}^{0}$	initial package concentration of gas species i ($kg \cdot m^{-3}$)
$C_{i,p}^{t}$	package concentration of gas species i at time t ($kg \cdot m^{-3}$)
$C_{N_2,\ e}$	N_2 concentration in the store atmosphere ($kg\ N_2 \cdot m^{-3}$)
$C_{N_2,\ p}$	N_2 concentration in the package atmosphere ($kg\ N_2 \cdot m^{-3}$)
$C_{O_2,\ f}$	O_2 concentration in the fruit internal atmosphere ($kg\ O_2 \cdot m^{-3}$)
$C_{O_2,\ e}$	O_2 concentration in the store atmosphere ($kg\ O_2 \cdot m^{-3}$)
$C_{O_2,\ p}$	O_2 concentration in the package atmosphere ($kg\ O_2 \cdot m^{-3}$)
D	mass diffusivity ($m^2 \cdot s^{-1}$)
$D_{i,\ eff}$	effective diffusivity of gas species i through holes in the packaging film ($m^2 \cdot s^{-1}$)
$D_{i,\ ref}$	diffusivity of gas species i in air at temperature T_{ref} ($m^2 \cdot s^{-1}$)
$D_{i,\ air}$	diffusivity of gas species i in air ($m^2 \cdot s^{-1}$)
$D_{CO_2,\ eff}$	effective diffusivity of CO_2 through holes in the packaging film ($m^2 \cdot s^{-1}$)
$D_{H_2O,\ eff}$	effective diffusivity of water vapour through holes in the packaging film ($m^2 \cdot s^{-1}$)

$D_{N_2, eff}$	effective diffusivity of N_2 through holes in the packaging film ($m^2 \cdot s^{-1}$)
$D_{O_2, eff}$	effective diffusivity of O_2 through holes in the packaging film ($m^2 \cdot s^{-1}$)
$E_{a, i}$	activation energy for permeation of gas species i ($J \cdot mol^{-1}$)
h	surface heat transfer coefficient ($W \cdot m^{-2} \cdot K^{-1}$)
h_e	convective heat transfer coefficient at the external package surface ($W \cdot m^{-2} \cdot K^{-1}$)
h_f	convective heat transfer coefficient at the fruit surface ($W \cdot m^{-2} \cdot K^{-1}$)
h_{fg}	latent heat of vaporization of water ($J \cdot kg^{-1}$)
h_p	convective heat transfer coefficient at the internal packaging-film surface ($W \cdot m^{-2} \cdot K^{-1}$)
H_p	absolute humidity of the package atmosphere ($kg \cdot kg^{-1}$)
k	general rate constant (units variable)
k_{CO_2}	fruit skin permeance to CO_2 ($m \cdot s^{-1}$)
k_{O_2}	fruit skin permeance to O_2 ($m \cdot s^{-1}$)
$k_{g, skin}$	fruit skin permeance to water vapour ($s \cdot m^{-1}$)
$k_{g, tray}$	mass transfer coefficient for moisture sorption at the tray surface ($s \cdot m^{-1}$)
$k_{g, fruit}$	mass transfer coefficient for moisture condensation at the fruit surface ($s \cdot m^{-1}$)
$k_{g, film}$	mass transfer coefficient for moisture condensation at the inside surface of the packaging film ($s \cdot m^{-1}$)
k_{ic}	competitive inhibition constant (kg $CO_2 \cdot m^{-3}$)
k_{iu}	uncompetitive inhibition constant (kg $CO_2 \cdot m^{-3}$)
k_m	half saturation constant (kg $O_2 \cdot m^{-3}$)
K	parameter of the GAB isotherm model (Eq. 2.22)
L	characteristic dimension (m)
$\dot{m}_i$	net mass flow of gas species i into the package by all mechanisms except bulk flow ($mol \cdot s^{-1}$)
$\dot{m}_{CO_2}$	net mass flow of CO_2 into the package through fruit gas exchange, permeation, and diffusion ($kg \cdot s^{-1}$)
$\dot{m}_{H_2O}$	net mass flow of H_2O into the package through fruit moisture loss, permeation, diffusion, condensation/evaporation, and sorption/desorption ($kg \cdot s^{-1}$)
$\dot{m}_{N_2}$	net mass flow of N_2 into the package through permeation and diffusion ($kg \cdot s^{-1}$)
$\dot{m}_{O_2}$	net mass flow of O_2 into the package through fruit gas exchange, permeation, and diffusion ($kg \cdot s^{-1}$)
$M_{i, p}$	mass of gas species i in the package atmosphere (kg)
$M_{CO_2, p}$	mass of CO_2 in the package atmosphere (kg)
$M_{H_2O, p}$	mass of water vapour in the package atmosphere (kg)
$M_{N_2, p}$	mass of N_2 in package atmosphere (kg)
$M_{O_2, p}$	mass of O_2 in package atmosphere (kg)
$M_{cond, f}$	mass of condensate on the fruit surface (kg)
$M_{cond, p}$	mass of condensate on the inside packaging film surface (kg)
$M_{f, initial}$	initial total fruit mass (kg)
M_f	total fruit mass (kg)
M_n	individual fruit mass (kg)
M_p	mass of dry air in the package atmosphere (kg)
M_{tray}	tray dry mass ($kg \cdot tray^{-1}$)
$M_{w, tray}$	mass of water absorbed by the moulded-pulp trays ($kg \cdot tray^{-1}$)
Mr_i	molecular mass of gas species i ($g \cdot mol^{-1}$)
Mr_C	molar mass of carbon ($g \cdot mol^{-1}$)

Mr_{CO_2}	molar mass of CO_2 ($g \cdot mol^{-1}$)
Mr_{H_2O}	molar mass of water ($g \cdot mol^{-1}$)
Mr_{N_2}	molar mass of N_2 ($g \cdot mol^{-1}$)
Mr_{O_2}	molar mass of O_2 ($g \cdot mol^{-1}$)
n_h	total molar flow into the package through holes in the packaging film ($mol \cdot s^{-1}$)
$\dot{n}_i$	net molar flow of gas species i into the package by all mechanisms except bulk flow ($mol \cdot s^{-1}$)
$\dot{n}_{CO_2}$	net molar flow of CO_2 into the package through fruit gas exchange, permeation, and diffusion ($mol \cdot s^{-1}$)
$\dot{n}_{H_2O}$	net molar flow of H_2O into the package through fruit moisture loss, permeation, diffusion, condensation/evaporation, and sorption/desorption ($mol \cdot s^{-1}$)
$\dot{n}_{N_2}$	net molar flow of N_2 into the package through permeation and diffusion ($mol \cdot s^{-1}$)
$\dot{n}_{O_2}$	net molar flow of O_2 into the package through fruit gas exchange, permeation, and diffusion ($mol \cdot s^{-1}$)
$n_{p,tot}$	total number of moles of gas in the package atmosphere
N	number of fruit in the package
N_{tray}	number of moulded-pulp trays per package
$p_{sat,tray}$	saturated vapour pressure of water at the tray temperature (Pa)
$p_{sat,film}$	saturated vapour pressure of water at the packaging film temperature (Pa)
$p_{sat,f}$	saturated vapour pressure of water at the fruit surface temperature (Pa)
$p_{sat,e}$	saturated vapour pressure of water at the store air temperature (Pa)
$p_{sat,p}$	saturated vapour pressure of water at the temperature of the package atmosphere (Pa)
$p_{w,tray}$	partial pressure of water vapour at the tray surface (Pa)
$p_{w,f}$	partial pressure of water vapour beneath the fruit skin (Pa)
$p_{w,e}$	partial pressure of water vapour in the store atmosphere (Pa)
$p_{w,p}$	partial pressure of water vapour in the package atmosphere (Pa)
P	pressure (Pa)
$P_{0,i}$	pre-exponential factor for permeation of gas species i ($m^2 \cdot s^{-1}$)
P_{atm}	atmospheric pressure (Pa)
P_i	permeability of the packaging film to gas species i ($m^2 \cdot s^{-1}$)
P_{CO_2}	packaging film permeability to CO_2 ($m^2 \cdot s^{-1}$)
P_{H_2O}	packaging film permeability to water vapour ($m^2 \cdot s^{-1}$)
P_{N_2}	packaging film permeability to N_2 ($m^2 \cdot s^{-1}$)
P_{O_2}	packaging film permeability to O_2 ($m^2 \cdot s^{-1}$)
P_p	package atmosphere pressure (Pa)
Q	cumulative O_2 consumption ($kg\ O_2 \cdot kg^{-1}$)
Q_{10}	temperature coefficient for respiration
R	gas constant ($J \cdot mol^{-1} \cdot K^{-1}$)
RH_e	relative humidity of the store air (%)
RH_p	relative humidity of the package atmosphere (%)
RQ_m	mass-based respiratory quotient for aerobic respiration ($kg \cdot kg^{-1}$)
SA_{corr}	empirical correction factor for evaporation of moisture from the fruit surface
t	time (s)
$t_{0.5}$	half cooling or warming time or half life (s)
t_h	time at which holes in the packaging film are formed (s)

T	temperature (K)
T_{ref}	reference temperature (K)
U_{pack}	overall heat transfer coefficient for the packaging materials ($W \cdot m^{-2} \cdot K^{-1}$)
v	aerobic respiration rate (kg $O_2 \cdot kg^{-1} \cdot s^{-1}$)
v_{max}	maximum aerobic respiration rate at the fruit temperature (kg $O_2 \cdot kg^{-1} \cdot s^{-1}$)
$v_{max,ref}$	maximum aerobic respiration rate at the reference temperature (kg $O_2 \cdot kg^{-1} \cdot s^{-1}$)
V_{carton}	carton volume (m^3)
$V_{i,p}$	volume of gas species i in the package atmosphere (m^3)
$V_{CO_2,p}$	volume of CO_2 in the package atmosphere (m^3)
$V_{H_2O,p}$	volume of water vapour in the package atmosphere (m^3)
$V_{N_2,p}$	volume of N_2 in the package atmosphere (m^3)
$V_{O_2,p}$	volume of O_2 in the package atmosphere (m^3)
V_n	individual fruit volume (m^3)
$V_{p,min}$	minimum package atmosphere volume (m^3)
V_p	volume of the package atmosphere (m^3)
$V_{p,h}$	package atmosphere volume at time t_h (m^3)
W	respiratory heat generation per unit mass of O_2 consumption ($J \cdot kg^{-1}$)
x	packaging film thickness (m)
x_i	thickness of the i^{th} layer of packaging material (m)
X_i	mole fraction of gas species i in the bulk flow through holes in the packaging film
X_{CO_2}	mole fraction of CO_2 in the flow through holes in the packaging film
X_{H_2O}	mole fraction of water vapour in the flow through holes in the packaging film
X_{N_2}	mole fraction of N_2 in the flow through holes in the packaging film
X_{O_2}	mole fraction of O_2 in the flow through holes in the packaging film
$X_{CO_2,e}$	mole fraction of CO_2 in the store air (dry air basis)
$X_{N_2,e}$	mole fraction of N_2 in the store air (dry air basis)
$X_{O_2,e}$	mole fraction of O_2 in the store air (dry air basis)
X_m	parameter of the GAB isotherm model (Eq. 2.22)
X_{tray}	tray moisture content on a dry solids basis ($kg \cdot kg^{-1}$)
Y	fractional unaccomplished temperature change
Y_i'	fractional unaccomplished concentration change for gas species i
$[i]$	volume concentration of gas species i ($m^3 \cdot m^{-3}$)
$[i]_e$	volume concentration of gas species i in the store atmosphere ($m^3 \cdot m^{-3}$)
$[i]_p$	volume concentration of gas species i in the package atmosphere ($m^3 \cdot m^{-3}$)
$[CO_2]_e$	volume concentration of CO_2 in the store atmosphere ($m^3 \cdot m^{-3}$)
$[H_2O]_e$	volume concentration of water vapour in the store atmosphere ($m^3 \cdot m^{-3}$)
$[H_2O]_p$	volume concentration of water vapour in the package atmosphere ($m^3 \cdot m^{-3}$)
$[N_2]_e$	volume concentration of N_2 in the store atmosphere ($m^3 \cdot m^{-3}$)
$[O_2]_e$	volume concentration of O_2 in the store atmosphere ($m^3 \cdot m^{-3}$)

α	constant in Eq. 6.82 (s^{-1})
γ	constant in Eq. 6.82
ε	fruit flesh porosity ($m^3 \cdot m^{-3}$)
η_f	fruit specific enthalpy ($J \cdot kg^{-1}$)
η_p	specific enthalpy of the package atmosphere (dry air basis) ($J \cdot kg^{-1}$)
η_{tray}	specific enthalpy of the moulded-pulp fruit trays (dry mass basis) ($J \cdot kg^{-1}$)

θ	temperature (°C)
θ_e	store air temperature (°C)
θ_f	fruit temperature (°C)
θ_{film}	temperature of the packaging film (°C)
θ_i	initial temperature (°C)
θ_p	temperature of the package atmosphere (°C)
θ_{ref}	reference temperature (°C)
λ	thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)
λ_i	thermal conductivity of the i^{th} layer of packaging material ($W \cdot m^{-1} \cdot K^{-1}$)
ξ	empirical correction factor for gas diffusion through holes
$\rho_{f,\,initial}$	initial fruit flesh density ($kg \cdot m^{-3}$)
ρ_f	fruit flesh density ($kg \cdot m^{-3}$)