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Mathematical Modelling of Mass Transfer in Food Packaging Systems

A thesis presented in partial fulfilment of the requirements for the degree of
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ABSTRACT

Food packaging is of critical importance for New Zealand food exports. One function of food packaging is to preserve the quality of food products during shipping and distribution, a key aspect of which is the control of mass transfer (in particular moisture). As such moisture transfer is an important consideration in the design of food packaging. However traditional food packaging selection has often involved a quantitative or “trial and error” approach. Mathematical models present a useful alternative, allowing changes to current system properties as well as the design of new systems to be investigated prior to physical testing. The objectives of this study were to: investigate the processes and considerations involved in food packaging selection, formulate mathematical models that can be used to predict moisture transfer in food packaging systems, and present potential applications for the developed mathematical models.

To obtain a broad understanding of food packaging, the properties of common packaging materials used in the food industry as well as current consumer and technological trends were reviewed. Considerations involved in food packaging selection were then investigated, including general considerations followed by a focus on mass transfer and barrier properties. It was found that, although theory allowing the quantitative selection of food packaging barrier properties is fairly comprehensive, it is common industry practice to select packaging qualitatively. This suggested that many food packaging systems are sub-optimised. Several phenomena not generally considered in food packaging selection were also investigated as required for the formulation of the mathematical models.

Review of literature revealed significant gaps regarding data of food packaging barrier properties. Therefore, to assist with the identification of specific applications for the mathematical models, a summary of the barrier property requirements of various food products was produced. As part of this work a table of the barrier properties of food packaging materials presented in a standard format was compiled.

Mathematical models were developed describing various mass transfer processes in food packaging systems. Firstly moisture transfer in a standard food package system was considered, consisting of a food product enclosed in a single individual packaging layer which may contain perforations. Further models were developed extending the standard system to include systems with two individual packaging layers that each may contain perforations, as well as packages containing food powders where mass transfer in the food powder is also significant. Systems with perforations in contact with food powder or centred on a relatively small isolated air pocket were also considered, where a localised two-dimensional moisture profile results. Finally, a food package consolidation model was developed to allow optimisation of such systems. Formulation of each model involved development of a conceptual system (including the identification of key processes and properties, and specifying assumptions), formulation of a mathematical model, a numerical or analytical solution using MATLAB® software, and validation against experimental observations.

Several potential applications for the developed mathematical models were identified. A particular focus was placed on food powder systems with perforated packaging, such as those for which dense phase filling is used. This may include flours, sugar, soy powders, dairy powders, and other industrial or commercial food ingredients. Many high moisture content food products were also identified as having conceptually similar packaging systems, such as fresh produce, dairy products, meat products, and seafood. However it was noted that some extensions to the mathematical models may be required in some cases.

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NOMENCLATURE

A_{bag} = Surface area of paperboard bag (m^{2})

A_{f} = Surface area of food powder (m^{2})

$A_{f,air}$ = Area of air pocket in contact with food powder (m^{2})

$A_{f,r}$ = Area of node in radial direction (m^{2})

$A_{f,x}$ = Area of node in axial direction (m^{2})

$A_{f,x,air}$ = Area of node in axial direction in contact with air pocket (m^{2})

A_{lnr} = Surface area of polymer liner (m^{2})

A_{pkg} = Package surface area (m^{2})

$A_{prf,bag}$ = Total area of perforation(s) in paperboard bag (m^{2})

A_{prf} = Total area of perforation(s) in packaging (m^{2})

$A_{prf,lnr}$ = Total area of perforation(s) in polymer liner (m^{2})

A_{stk} = Contact area of mass stacked on top of food package (m^{2})

b_{lin} = Slope of linear isotherm of food (-)

C_{BET} = Guggenheim constant for BET isotherm of food (-)

C_{GAB} = Guggenheim constant for GAB isotherm of food (-)

c_{lin} = Constant for linear isotherm of food ((kg water).(kg solids)$^{-1)}$

$D_{0,bag,n}^{H_2O}$ = Pre-exponential factor of diffusivity of water vapour in nth layer of paperboard bag (m^{2}.s^{-1})

$D_{0,lnr,n}^{H_2O}$ = Pre-exponential factor of diffusivity of water vapour in nth layer of polymer liner (m^{2}.s^{-1})

$D_{0,pkg,n}^{H_2O}$ = Pre-exponential factor of diffusivity of water vapour in nth layer of packaging (m^{2}.s^{-1})

$D_{air}^{H_2O}$ = Diffusivity of water vapour in air (m^{2}.s^{-1})

$D_{bag,n}^{H_2O}$ = Diffusivity of water vapour in nth layer of paperboard bag (m^{2}.s^{-1})

$D_{eff}^{H_2O}$ = Effective diffusivity of water vapour in food powder (m^{2}.s^{-1})

$D_{lnr,n}^{H_2O}$ = Diffusivity of water vapour in nth layer of polymer liner (m^{2}.s^{-1})

$D_{pkg,n}^{H_2O}$ = Diffusivity of water vapour in nth layer of packaging (m^{2}.s^{-1})

d_{prf} = Average diameter of perforations (m)

$d_{prf,bag}$ = Average diameter of perforation(s) in paperboard bag (m)

$d_{prf,lnr}$ = Average diameter of perforation(s) in polymer liner (m)

$D_{ref,bag,n}^{H_2O}$ = Reference diffusivity of water vapour in nth layer of paperboard bag (m^2.s^{-1})

$D_{ref,lnr,n}^{H_2O}$ = Reference diffusivity of water vapour in nth layer of polymer liner (m^2.s^{-1})

$D_{ref,pkg,n}^{H_2O}$ = Reference diffusivity of water vapour in nth layer of packaging (m^2.s^{-1})

$E_{D,lnr,n}^{H_2O}$ = Activation energy of diffusion of water vapour in nth layer of polymer liner (J.mol^{-1})

$E_{D,pkg,n}^{H_2O}$ = Activation energy of diffusion of water vapour in nth layer of packaging (J.mol^{-1})

$E_{D,bag,n}^{H_2O}$ = Activation energy of diffusion of water vapour in nth layer of paperboard bag (J.mol^{-1})

$E_{P,bag,n}^{H_2O}$ = Activation energy of permeation of water vapour in nth layer of paperboard bag (J.mol^{-1})

$E_{P,lnr,n}^{H_2O}$ = Activation energy of permeation of water vapour in nth layer of polymer liner (J.mol^{-1})

$E_{P,pkg,n}^{H_2O}$ = Activation energy of permeation of water vapour in nth layer of packaging (J.mol^{-1})

g = Acceleration due to gravity (m.s^{-1})

J = Total number of nodes per layer (-)

j = Node number (-)

$J_{prf}^{H_2O}$ = Diffusive flux of water vapour through perforation(s) in packaging (mol.m^{-2}.s^{-1})

$J_{prf,bag}^{H_2O}$ = Diffusive flux of water vapour through perforation(s) in paperboard bag (mol.m^{-2}.s^{-1})

$J_{prf,lnr}^{H_2O}$ = Diffusive flux of water vapour through perforation(s) in polymer liner (mol.m^{-2}.s^{-1})

K = Total number of nodes in radial direction of food powder (-)

k = Node number in radial direction (-)

K_{air} = Node number in radial direction positioned at edge of air pocket (-)

k_{GAB} = Constant for GAB isotherm of food (-)

M = Moisture content of food ((kg water).(kg solids)$^{-1}$)

$M_{0,GAB}$ = Moisture content of monolayer for GAB isotherm ((kg water).(kg solids)$^{-1}$)

$M_{0,GAB}$ = Moisture content of monolayer for GAB isotherm of food ((kg water).(kg solids)$^{-1}$)

$M_{1,BET}$ = Moisture content of monolayer for BET isotherm of food ((kg water).(kg solids)$^{-1}$)

M_i = Initial moisture content of food product ((kg water).(kg solids)$^{-1}$)

$M_{r,air}$ = Molecular mass of dry air (kg.mol^{-1})

M_{r,H_2O} = Molecular mass of water (kg.mol^{-1})

m_s = Mass of solids in food product (kg)

m_{stk} = Mass stacked on top of food package (kg)

N = Total number of packaging layers (-)

N_{bag} = Total number of layers in paperboard bag (-)

N_{lnr} = Total number of layers in polymer liner (-)

$p_0^{H_2O}$ = Saturated water vapour pressure (Pa)

$P_{0,bag,n}^{H_2O}$ = Pre-exponential factor of permeability of water vapour in n^th^ layer of paperboard bag (mol.m.m^{-2}.s^{-1}.Pa^{-1})

$P_{0,lnr,n}^{H_2O}$ = Pre-exponential factor of permeability of water vapour in nth layer of polymer liner (mol.m.m^{-2}.s^{-1}.Pa^{-1})

$P_{0,pkg,n}^{H_2O}$ = Pre−exponential factor of permeability of water vapour in nth layer of packaging (mol.m.m^{-2}.s^{-1}.Pa^{-1})

$p_a^{H_2O}$ = Water vapour pressure in ambient air (Pa)

$p_{ap}^{H_2O}$ = Water vapour pressure in air pocket (Pa)

p_{atm} = Atmospheric pressure (Pa)

$p_{bag}^{H_2O}$ = Water vapour pressure in paperboard bag (Pa)

$p_{bag,i}^{H_2O}$ = Initial water vapour pressure in paperboard bag (Pa)

$P_{bag,n}^{H_2O}$ = Permeability of water vapour in nth layer of paperboard bag (mol.m.m^{-2}.s^{-1}.Pa^{-1})

$p_{bh}^{H_2O}$ = Water vapour pressure in bag headspace (Pa)

$p_f^{H_2O}$ = Water vapour pressure in food (Pa)

$p_{f,i}^{H_2O}$ = Initial water vapour pressure in food (Pa)

$p_{lh}^{H_2O}$ = Water vapour pressure in liner headspace (Pa)

$p_{lnr,i}^{H_2O}$ = Initial water vapour pressure in polymer liner (Pa)

$p_{lnr,j}^{H_2O}$ = Water vapour pressure in jth node of polymer liner (Pa)

$P_{lnr,n}^{H_2O}$ = Permeability of water vapour in nth layer of polymer liner (mol.m.m^{-2}.s^{-1}.Pa^{-1})

p_{ph}^{air} = Pressure of air in package headspace (Pa)

$p_{pkg}^{H_2O}$ = Water vapour pressure in packaging (Pa)

$p_{pkg,i}^{H_2O}$ = Initial water vapour pressure in packaging (Pa)

$P_{pkg,n}^{H_2O}$ = Permeability of water vapour in nth layer of packaging (mol.m.m^{-2}.s^{-1}.Pa^{-1})

R = Ideal gas constant (8.314 m^{3}.Pa.K^{-1}.mol^{-1} or J.K^{-1}.mol^{-1})

r = Spatial position in food powder in radial direction (m)

R_f = Thickness of food powder in radial direction (m)

RH_a = Ambient relative humidity (%)

$S_{0,bag,n}^{H_2O}$ = Pre-exponential factor of solubility of water vapour in nth layer of paperboard bag (mol.m^{-3}.Pa^{-1})

$S_{0,lnr,n}^{H_2O}$ = Pre-exponential factor of solubility of water vapour in nth layer of polymer liner (mol.m^{-3}.Pa^{-1})

$S_{0,pkg,n}^{H_2O}$ = Pre−exponential factor of solubility of water vapour in nth layer of packaging (mol.m^{-3}.Pa^{-1})

$S_{air}^{H_2O}$ = Solubility of water vapour in air (mol.m^{-3}.Pa^{-1})

$S_{bag,n}^{H_2O}$ = Solubility of water vapour in nth layer of paperboard bag (mol.m^{-3}.Pa^{-1})

$S_{f}^{H_2O}$ = Solubility of water vapour in food powder (mol.m^{-3}.Pa^{-1})

$S_{lnr,n}^{H_2O}$ = Solubility of water vapour in nth layer of polymer liner (mol.m^{-3}.Pa^{-1})

$S_{pkg,n}^{H_2O}$ = Solubility of water vapour in nth layer of packaging (mol.m^{-3}.Pa^{-1})

$S_{ref,bag,n}^{H_2O}$ = Reference solubility of water vapour in nth layer of paperboard bag (mol.m^{-3}.Pa^{-1})

$S_{ref,lnr,n}^{H_2O}$ = Reference solubility of water vapour in nth layer of polymer liner (mol.m^{-3}.Pa^{-1})

$S_{ref,pkg,n}^{H_2O}$ = Reference solubility of water vapour in nth layer of packaging (mol.m^{-3}.Pa^{-1})

T = Temperature (K)

t = Time (s)

$T_{ref,D_{bag}^{H_2O},n}$ = Temperature of reference diffusivity of water vapour in nth layer of paperboard bag (K)

$T_{ref,D_{lnr}^{H_2O},n}$ = Temperature of reference diffusivity of water vapour in nth layer of polymer liner (K)

$T_{ref,D_{pkg}^{H_2O},n}$ = Temperature of reference diffusivity of water vapour in nth layer of packaging (K)

$T_{ref,S_{bag}^{H_2O},n}$ = Temperature of reference solubility of water vapour in nth layer of paperboard bag (K)

$T_{ref,S_{lnr}^{H_2O},n}$ = Temperature of reference solubility of water vapour in nth layer of polymer liner (K)

$T_{ref,S_{pkg}^{H_2O},n}$ = Temperature of reference solubility of water vapour in nth layer of packaging (K)

V_{air} = Volume of air in package headspace (m^3)

x = Spatial position (m)

$X_{bag,n}$ = Thickness of nth layer of paperboard bag (m)

X_f = Thickness of food powder (m)

$X_{lnr,n}$ = Thickness of nth layer of polymer liner (m)

X_n = Thickness of nth layer of packaging (m)

X_T = Total thickness of packaging (m)

$X_{T,bag}$ = Total thickness of paperboard bag (m)

$X_{T,lnr}$ = Total thickness of polymer liner (m)

$X_{T,pkg}$ = Total thickness of packaging (m)

$\Delta H_{S,bag,n}^{H_2O}$ = Partial molar enthalpy of sorption of water vapour in nth layer of paperboard bag ($J.mol^{-1}$)

$\Delta H_{S,lnr,n}^{H_2O}$ = Partial molar enthalpy of sorption of water vapour in nth layer of polymer liner ($J.mol^{-1}$)

$\Delta H_{S,pkg,n}^{H_2O}$ = Partial molar enthalpy of sorption of water vapour in nth layer of packaging ($J.mol^{-1}$)

Δr_f = Width of node in radial direction of food powder (m)

$\Delta x_{bag,n}$ = Width of node in nth layer of paperboard bag (m)

Δx_{f} = Width of node in food powder (m)

$\Delta x_{lnr,n}$ = Width of node in nth layer of polymer liner (m)

$\Delta x_{pkg,n}$ = Width of node in nth layer of packaging (m)

ε = Porosity of food powder (-)

ρ_{air} = Density of air (kg.m^{3})

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