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Mathematical Modelling of Active Packaging Systems for Horticultural Products

**A thesis presented in partial fulfilment of the requirements for the degree of
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at Massey University, New Zealand**

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ABSTRACT

Active packaging systems can offer significant advantages in preventing quality loss in horticultural products through control of microbial and/or physiological activity. By delivering and sustaining volatile active agents at effective levels in a package atmosphere, significant shelf life extension can thus be achieved. Design of these systems is complicated by the number of possible package, product, active agent and carrier combinations that can be employed and the significant interactions that may occur between these components. Mathematical modelling can be used to simplify system design and reduce the number of experimental trials required to achieve optimal active packaging systems. In this study a generalised modelling methodology was developed and validated to facilitate the design of active controlled volatile release packaging systems for horticultural products.

The modelling methodology was developed using an example system which comprised tomatoes packed under a modified atmosphere (MA; 5 % (v/v) CO₂ and 10 % (v/v) O₂) in a LDPE bag with a polymer film sealed sachet containing silica gel pre-saturated with the antifungal agent hexanal. Experimental trials showed that for this system a target sustained hexanal concentration of 40-70 ppm was required. This was shown to be (i) the minimum inhibitory concentration (MIC) for controlling *Botrytis cinerea* growing on tomatoes stored at 20°C and ~99%RH, (ii) to have only a relatively minor influence on the postharvest quality of tomatoes under these active MA conditions, and (iii) to promote only a small apparent uptake of hexanal from the atmosphere by the tomatoes.

The effective hexanal permeabilities of Tyvek[®], LDPE and OPP sachet films were characterised using the isostatic method and shown to exhibit a dependence on both temperature (10 and 20°C) and concentration (over a range of 0.01-0.22 mol·m⁻³). Average permeabilities decreased in the order of Tyvek[®] > LDPE > OPP, respectively, at all temperatures at comparable hexanal partial pressures.

Hexanal sorption isotherms for silica gel at both 10 and 20°C were determined using the gravimetric method and were reasonably well described by the Langmuir equation. The equilibrium amount adsorbed was significantly reduced at the higher temperature but the

pre-adsorption of water vapour on hexanal uptake on silica gel showed no uniform trend on the sorption characteristics suggesting that multicomponent sorption is complex.

A generalised modelling methodology was developed through conceptualising key mass transfer processes involved in these active MA packaging systems. Quantitative methods for deciding the relative importance of each process were established together with guidelines for when simplifying assumptions could be made. This information was formalised into a decision tree to allow appropriate assumptions to be made in model formulation without unacceptable loss of model accuracy. Methods to develop generalised equations from these assumptions to describe changes in the sachet, package headspace and outer bag film with respect to an active agent and MA gases were then identified.

The mathematical modelling methodology was applied to the example hexanal release active MAP tomato packaging system. For these systems there was a high initial peak in package headspace concentration during the first 24 h which declined to a quasi steady-state concentration over a period of days. The quasi steady-state headspace concentrations were generally in the MIC range and were well predicted by the model. Interactions between water vapour and silica gel may have been responsible for the relatively higher hexanal concentration at the onset of release from the Tyvek[®] sachet (a highly porous material). However the influence of water vapour (>95% RH in the MA bag containing tomatoes) during the quasi steady-state period appeared to be insignificant for all sachet films.

The model was successfully applied to a range of packaging configurations and storage temperatures. A lack of fit was evident between model predictions and experimental trials during the initial (unsteady-state) stages of the release pattern for both headspace vapour concentrations and adsorbed mass on the silica gel. These differences were attributed to (i) model input uncertainties, chiefly with regard to the estimated coefficients of both the Langmuir isotherm equation and film permeability, and (ii) overestimated effective permeability values predicted by extrapolation of the concentration dependence of film permeability beyond the conditions for which the permeability was measured. These results suggest improved models for the effective permeabilities of the films, quantified under a range of vapour concentrations and concentration gradients, are required for better describing fluxes across the sachet film.

Despite these limitations, the model did describe the general release pattern. The model was then used to pose a range of ‘*what-if*’ scenarios investigating the release patterns predicted for different active packaging designs. This analysis gave useful insights into how sorption isotherm shape and package/sachet design parameters can be manipulated to achieve different volatile release platforms.

The work clearly demonstrated the importance of accurate data for permeability of volatile compounds through polymer films and for sorption of the active agent on the carrier phase. More work on characterising these systems is recommended to further improve model-based design methods for active MAP systems.

Overall the generalised methodology developed can be confidently adopted for constructing a mathematical model that provides sufficient accuracy and simplicity to be implemented for designing active packaging systems for horticultural and food products.

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Table of contents

| | |
|---|---------------|
| Abstract..... | i |
| Acknowledgements | v |
| List of Nomenclatures..... | xv |
| List of Figures..... | xxiii |
| List of Tables | xxxiii |
| Chapter 1 | 1-1 |
| Introduction..... | 1-1 |
| 1.1 Background..... | 1-1 |
| 1.2 Research aim..... | 1-3 |
| 1.3 Research objectives..... | 1-3 |
| 1.4 Structure of thesis | 1-4 |
| Chapter 2 | 2-1 |
| Literature review | 2-1 |
| 2.1 Introduction..... | 2-1 |
| 2.2 Overview of active packaging technologies for horticultural products..... | 2-1 |
| 2.2.1 Active packaging requirements for horticultural products | 2-1 |
| 2.2.2 Oxygen-scavengers..... | 2-2 |
| 2.2.3 Carbon dioxide-scavengers or emitters, and dual-active systems | 2-2 |
| 2.2.4 Atmospheric control via temperature compensating films..... | 2-3 |
| 2.2.5 Water vapour regulators..... | 2-4 |
| 2.2.6 Ethylene regulators | 2-5 |
| 2.2.7 Antimicrobial packaging..... | 2-6 |
| 2.2.8 Other interesting trends and developments..... | 2-8 |
| 2.3 Modelling active modified atmosphere packaging (Active MAP) for horticultural products..... | 2-9 |
| 2.4 Sorption isotherms of active agents..... | 2-11 |
| 2.5 Controlled release of active agents to the package atmosphere..... | 2-18 |
| 2.5.1 Desorption..... | 2-19 |

| | |
|--|------------|
| 2.5.1.1 Models based on diffusion resistance | 2-20 |
| 2.5.1.2 Models based on instantaneous mass transfer..... | 2-20 |
| 2.5.2 Diffusion through mass transfer controlling polymeric film structures..... | 2-22 |
| 2.6 Permeation through packaging materials..... | 2-27 |
| 2.6.1 Polymer film materials: non-perforated and perforated films | 2-27 |
| 2.6.2 Paper-based packaging materials | 2-29 |
| 2.7 Interactions of active agents and horticultural products | 2-30 |
| 2.8 Summary | 2-32 |
| Chapter 3 | 3-1 |
| The effects of active agents on postharvest quality: Hexanal vapour and tomato model system | 3-1 |
| 3.1 Introduction..... | 3-1 |
| 3.2 Antifungal activity of hexanal vapour and its effects on tomato physiology and quality..... | 3-3 |
| 3.2.1 Materials and methods | 3-3 |
| 3.2.2 Results and discussion | 3-7 |
| 3.3 Apparent rate of uptake of hexanal vapour by tomatoes | 3-14 |
| 3.3.1 Materials and methods | 3-15 |
| 3.3.2 Results and discussion | 3-16 |
| 3.4 Effects of modified atmosphere conditions on apparent rate of hexanal uptake by tomatoes | 3-21 |
| 3.4.1 Experimental settings..... | 3-21 |
| 3.4.2 Results and discussion | 3-23 |
| 3.5 Summary | 3-26 |
| Chapter 4 | 4-1 |
| Evaluating the physico-chemical properties of hexanal vapour and silica gel adsorbents for active packaging applications..... | 4-1 |
| 4.1 Introduction..... | 4-1 |
| 4.2 Determination of effective film permeability to hexanal vapour..... | 4-1 |
| 4.2.1 Experimental procedures | 4-3 |
| 4.2.2 Results and discussion, part I : Overall effective permeability and concentration dependent characteristics | 4-7 |

| | |
|---|------------|
| 4.2.3 Results and discussion, part II: Comparison of experimentally measured permeabilities with published data | 4-14 |
| 4.2.3.1 Tyvek® film | 4-14 |
| 4.2.3.2 OPP film | 4-15 |
| 4.2.3.3 LDPE film..... | 4-19 |
| 4.2.3.4 Concluding remarks from the comparison of experimental and literature data..... | 4-24 |
| 4.3 Determination of hexanal sorption isotherms for silica gel adsorbents..... | 4-24 |
| 4.3.1 Approaches for determining sorption isotherms..... | 4-25 |
| 4.3.2 Experimental procedures | 4-26 |
| 4.3.3 Preliminary validation of the gravimetric sorption method..... | 4-27 |
| 4.3.4 Hexanal sorption isotherms for silica gel adsorbents | 4-29 |
| 4.3.5 Determinations of the effects of relative humidity on hexanal sorption..... | 4-34 |
| 4.4 Summary | 4-37 |
| Chapter 5 | 5-1 |
| Development of conceptual and mathematical models for active MAP of horticultural products | 5-1 |
| 5.1 Introduction..... | 5-1 |
| 5.2 Conceptual model of an active MAP system for horticultural products..... | 5-2 |
| 5.3 Assumptions for conceptual model development..... | 5-4 |
| 5.4 Primary (P) level assumptions | 5-4 |
| 5.4.1 Assumption P1: The gas phase of the active packaging system can be considered as ideal | 5-4 |
| 5.4.2 Assumption P2: All model compartments are in local thermal equilibrium | 5-4 |
| 5.4.3 Assumption P3: Mass transfer of the active agent from the sachet can be modelled in 1-dimension | 5-5 |
| 5.4.4 Assumption P4: Uniform concentrations of active agents in the package headspace | 5-5 |
| 5.4.5 Assumption P5: Negligible contribution of active agent accumulation to changes in package volume and total pressure | 5-7 |
| 5.5 Secondary level assumptions | 5-8 |
| 5.5.1 Modelling of controlled release sachet systems (r_{scfl}^i)..... | 5-9 |
| 5.5.1.1 Modelling mass transfer within the active agent carrier..... | 5-9 |

| | |
|--|------------|
| 5.5.1.2 Modelling mass transfer across the sachet film material | 5-11 |
| 5.5.2 Modelling packaging film material (r_{pkfl}^i) | 5-17 |
| 5.5.3 Modelling the active agent interaction with the product (r_{fr}^i) | 5-20 |
| 5.5.4 Modelling accumulation in the package headspace (r_{pkhs}^i) | 5-22 |
| 5.6 A comprehensive decision tree for the design of active packaging system for horticultural products | 5-24 |
| 5.7 Mathematical model formulation for the Hexanal/Silica gel/Tomato active MAP system | 5-27 |
| 5.7.1 Rate of hexanal release from sachet | 5-27 |
| 5.7.2 Rate of hexanal transfer across the packaging film material | 5-28 |
| 5.7.3 Apparent rate of hexanal uptake by tomatoes | 5-30 |
| 5.7.4 Rate of accumulation of CO ₂ and O ₂ in package headspace (passive MAP) .. | 5-30 |
| 5.8 Numerical solution of overall transport model | 5-31 |
| 5.8.1 MATLAB solver for numerical solutions | 5-31 |
| 5.8.2 Finite difference solutions for PDE models | 5-32 |
| 5.8.2.1 Explicit finite different scheme | 5-32 |
| 5.8.2.2 The grid and finite difference approximations | 5-33 |
| 5.8.2.3 ODE equations for film nodes | 5-33 |
| 5.8.2.3.1 For surfaces of the film (nodes $j = 1$ and $j = J+1$) | 5-33 |
| 5.8.2.3.2 For internal film (nodes $j = 2 : J$) | 5-34 |
| 5.8.3 The global mathematical model | 5-35 |
| 5.8.4 MATLAB [®] language codes | 5-36 |
| 5.8.5 Model checking: Checks against analytical solutions and numerical error checking | 5-36 |
| 5.9 Summary | 5-37 |
| Chapter 6 | 6-1 |
| Mathematical model validation | 6-1 |
| 6.1 Introduction | 6-1 |
| 6.2 Experiments used in validating the mathematical models | 6-1 |
| 6.3 Model input data and sensitivity analysis | 6-4 |
| 6.4 Experimental results and discussion of model performance | 6-6 |
| 6.4.1 Effects of sachet loading on the package headspace hexanal concentration | 6-6 |

| | |
|--|------------|
| 6.4.1.1 Model predictions for packages containing sealed glass jars | 6-6 |
| 6.4.1.2 Model predictions for packages containing tomatoes..... | 6-16 |
| 6.4.2 Effects of the ratio of sachet to package surface area (ω_A) on the package headspace hexanal concentrations | 6-22 |
| 6.4.3 Effects of the type of sachet film on the package headspace hexanal concentration..... | 6-23 |
| 6.4.3.1 OPP sachet film | 6-24 |
| 6.4.3.2 Tyvek [®] sachet film | 6-26 |
| 6.4.4 Effects of storage temperature on the package headspace hexanal concentrations | 6-30 |
| 6.4.5 Changes of hexanal adsorbed amount on silica gel..... | 6-37 |
| 6.4.5.1 Materials and methods | 6-37 |
| 6.4.5.2 Results and discussion | 6-38 |
| 6.5 Summary | 6-46 |
| Chapter 7 | 7-1 |
| Mathematical model applications..... | 7-1 |
| 7.1 Introduction..... | 7-1 |
| 7.2 Effects of isotherm types on hexanal release patterns | 7-1 |
| 7.3 Effects of isotherm shape on flux of hexanal across the sachet boundary | 7-14 |
| 7.3.1 Changes of flux as a function of isotherm shape..... | 7-14 |
| 7.3.2 Changes of flux as a function of time with regard to sorption isotherm shapes.. | 7-16 |
| 7.4 Conceptual designs of ethanol vapour active MAP systems | 7-19 |
| 7.5 Summary..... | 7-25 |
| Chapter 8 | 8-1 |
| General discussion and conclusions | 8-1 |
| 8.1 General discussion | 8-1 |
| 8.2 Conclusions..... | 8-9 |
| 8.3 Suggestions for future research..... | 8-10 |
| References..... | 9-1 |
| Appendix A..... | A-1 |

| | |
|--|------------|
| Active packaging technologies for horticultural produce | A-1 |
| Appendix B | B-1 |
| Hexanal reduces infection of tomatoes by <i>Botrytis cinerea</i> whilst maintaining quality | B-1 |
| Appendix C | C-1 |
| Gas chromatographic analysis procedures..... | C-1 |
| Appendix D | D-1 |
| Modelling mass transfer across film..... | D-1 |
| D.1 Derivations of mathematical models describing rate of hexanal release from sachet to package headspace | D-1 |
| D.2 Modelling concentration gradients and fluxes across experimentally utilised films . | D-4 |
| D.2.1 Modelling concentration gradients..... | D-4 |
| D.2.2 Modelling fluxes | D-4 |
| D.3 Alternative model describing the rate of hexanal release from sachet to package headspace (based on an assumption of the Langmuir relationship between hexanal vapour and LDPE film sorption)..... | D-5 |
| Appendix E | E-1 |
| Comparison of hexanal sorption isotherm for silica gel adsorbents estimated by different methods | E-1 |
| E.1 Verification using IGC techniques | E-1 |
| E.2 Isotherm determination by pulse IGC method | E-1 |
| E.2.1 Experimental procedures of pulse IGC | E-1 |
| E.2.2 Results and discussion of pulse IGC | E-2 |
| E.3 Isotherm determination by frontal IGC method | E-3 |
| E.3.1 Experimental procedures | E-3 |
| E.3.2 Results and discussion of FIGC..... | E-4 |
| E.4 Isotherm determinations by the volumetric sorption method..... | E-6 |
| E.4.1 Experimental procedures | E-6 |
| E.4.2 Results and discussion..... | E-6 |
| E.5 Linearisation of Langmuir model (following (Ratkowsky 1990))..... | E-11 |

| | |
|---|------------|
| E.6 Sorption isotherms of hexanal vapour for silica gel at 10 and 20°C (presented in molar units) | E-12 |
| Appendix F | F-1 |
| Formulation of global mathematical models..... | F-1 |
| F.1 Calculations of Bi values for hexanal mass transfer in sachet and package headspace F-1 | |
| F.2 Scaling analyses..... | F-1 |
| F.2.1 Scaling considered at sachet film material | F-2 |
| F.2.2 Scaling considered at packaging film..... | F-10 |
| F.3 Derivations of mathematical models for exploring the effects of capacity ratios ($CR_{pkhs/scfl}$ and $CR_{pkhs/pkfl}$; Chapter 5) on modelling 1-MCP accumulation in package headspace | F-16 |
| F.3.1 Modelling 1-MCP accumulation in package headspace based on ‘Modes of mass transfer across sachet film material’ | F-16 |
| F.3.2 Modelling 1-MCP accumulations in package headspace based on ‘Modes of mass transfer across packaging film material’ | F-18 |
| F.3.3 Numerical solutions for 1-MCP accumulation in package headspace investigations... .. | F-19 |
| F.4 Calculation of $CR_{bed/scfl}$, $CR_{pkhs/scfl}$, and $CR_{pkhs/pkfl}$ for hexanal-active MAP system | F-19 |
| Appendix G..... | G-1 |
| Numerical solutions | G-1 |
| G.1 Numerical solution for the global model describing hexanal concentration accumulation in the package headspace | G-1 |
| G.1.1 Function file (Hexanal_ActivePkgSim.m)..... | G-1 |
| G.1.2 Script file (Hexanal_ActivePkgSimrun.m)..... | G-2 |
| G.2 MATLAB® language for the global model for predicting accumulations of O ₂ and CO ₂ in active MAP for tomatoes | G-5 |
| G.2.1 Function file (PassiveMAP.m)..... | G-5 |
| G.2.2 Script file (PassiveMAPrun.m)..... | G-6 |
| G.2.3 Model inputs for simulations of O ₂ and CO ₂ | G-7 |

| | |
|--|------------|
| G.3 Analytical solution for mean hexanal vapour concentration in the packaging film (PDE modelling approach) | G-7 |
| G.4 Analytical solution for hexanal permeation across the sachet film (steady-state modelling approach) | G-10 |
| Appendix H..... | H-1 |
| Model validations | H-1 |
| H.1 Controlled release sachet preparations..... | H-1 |
| H.2 Summary of sensitivity analyses of model validations | H-2 |

LIST OF NOMENCLATURES

| | |
|----------------------------|---|
| A_{film} | = Film area (m^2) |
| A_{scfl} | = Sachet film surface area (m^2) |
| A_{pkfl} | = Packaging film surface area (m^2) |
| A_{fr} | = Fruit surface area (m^2) |
| a_{exp}^{Hxl} | = Coefficient of the hexanal exponential isotherm equation ($g \cdot g^{-1}$) |
| A_{GC}^i | = Area of gas chromatogram peak from the injected volume of sample (area) |
| b_{Lgm}^i | = Langmuir constant ($m^3 \cdot mol^{-1}$) |
| b_{film} | = Fitted exponential coefficient of effective permeability to hexanal of the film ($m^3 \cdot mol^{-1}$) |
| b_{Tyvek} | = Fitted exponential coefficient of effective permeability to hexanal of Tyvek [®] , LDPE and OPP films, respectively ($m^3 \cdot mol^{-1}$) |
| b_{LDPE} | |
| b_{OPP} | |
| $b_{Lgm,10^\circ C}^{Hxl}$ | = Langmuir coefficients at 10 and 20°C (dimensionless), respectively |
| $b_{Lgm,20^\circ C}^{Hxl}$ | |
| Bi | = Biot number for mass transfer (dimensionless) |
| b_{scfl} | = Fitted exponential model coefficient of effective permeability to hexanal vapour of sachet film material ($m^3 \cdot mol^{-1}$) |
| b_{Lgm}^{Hxl} | = Langmuir constant of hexanal sorption ($m^3 \cdot mol^{-1}$) |
| b_{pkfl} | = Fitted exponential model coefficient for effective permeability to hexanal vapour of packaging film material ($m^3 \cdot mol^{-1}$) |
| b_{exp}^{Hxl} | = Coefficient of the hexanal exponential isotherm equation (dimensionless) |
| $C_{gas\ phase}$ | = Equilibrium concentration in gas phase ($mol \cdot m^{-3}$) |
| C_{film}^i | = Concentration of the diffusant i in film ($mol \cdot m^{-3}$) |
| ΔC_{film}^i | = Concentration difference of diffusant i between the two sides of the film ($mol \cdot m^{-3}$) |
| C_g^i | = Equilibrium vapour concentration (or pressure) of adsorbate i with adsorbents (gas phase, $mol \cdot m^{-3}$) |

- C_s^i = Equilibrium adsorbed amount of adsorbate i on adsorbents (solid phase, $\text{mol}\cdot\text{g}^{-1}$)
- $C_{s,max}^i$ = Maximum adsorbed amount of adsorbate i on adsorbent estimated by Langmuir sorption isotherm ($\text{mol}\cdot\text{g}^{-1}$)
- C_{inlet}^{Hxl} = Inlet hexanal concentration ($\text{mol}\cdot\text{m}^{-3}$)
- C_{outlet}^{Hxl} = Outlet hexanal concentration ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{h,conc}^{Hxl}$,
 $C_{l,conc}^{Hxl}$ = Hexanal concentration at the high and low concentration side of the film, respectively ($\text{mol}\cdot\text{m}^{-3}$)
- C_{avg}^{Hxl} = Effective mean of hexanal concentrations measured in both chambers of the permeability cell at steady-state ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,x\ film}^{Hxl}$ = Hexanal concentration in the gas phase which is equilibrium with film at position x in film material (x_{film}) ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{paper\ phase}$ = Equilibrium concentration in paper phase ($\text{mol}\cdot\text{g}^{-1}$)
- $C_{scfl,0}^i$ = Concentration of active agent i in sachet film at $x = 0$, facing the carrier bed ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{scfl,Lscfl}^i$ = Concentration of active agent i in the sachet film at $x = L_{scfl}$, facing the package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{pkfl,0}^i$ = Concentration of active agent i in the film at $x = 0$, facing the package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{pkfl,Lpkfl}^i$ = Concentration of active agent i in the film at $x = L_{pkfl}$, facing the surrounding environment ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{fr,ext}^{O_2}$,
 $C_{fr,int}^{O_2}$ = Concentration of gas O_2 in external and internal fruit, respectively ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{fr}^{SO_2}$ = Concentration of SO_2 dissolved in fruit ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{fr,e}^{SO_2}$ = Equilibrium concentration representing the maximum SO_2 concentration attained in the corn ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{fr,air}^i$ = Concentration of active agent i surrounding fruit ($\text{mol}\cdot\text{m}^{-3}$)
- C_{pkhs}^i = Concentration of active agent i in package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,bed}^{Hxl}$ = Equilibrium hexanal vapour concentration above the carrier bed ($\text{mol}\cdot\text{m}^{-3}$)

- C_{pkhs}^{Hxl} = Hexanal vapour concentration in the package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- C_{sat}^{Hxl} = Saturated hexanal vapour concentration at a given temperature ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{s,bed}^{Hxl}$ = Equilibrium adsorbed amount of hexanal on the carrier bed ($\text{mol}\cdot\text{g}^{-1}$)
- $C_{s,max}^{Hxl}$ = Maximum amount of hexanal adsorbed on the carrier estimated by the Langmuir sorption isotherm ($\text{mol}\cdot\text{g}^{-1}$)
- C_{env}^{Hxl} = Hexanal concentration in the bulk environment surrounding the outer bag ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,1}^{Hxl}$,
 $C_{g,J+1}^{Hxl}$ = Equilibrium hexanal vapour concentration in the packaging film, at the discrete nodes $j = 1$ and $j = J + 1$, respectively ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,j}^{Hxl}$ = Equilibrium hexanal vapour concentration in the packaging film at discrete node $j = 2 : J$ ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{s,bed,i}^{Hxl}$ = Initial hexanal adsorbed amount of the carrier bed ($\text{mol}\cdot\text{g}^{-1}$)
- C^i = Concentration of VOC i ($\text{mol}\cdot\text{m}^{-3}$)
- C_{scfl}^{Hxl} = Hexanal concentration in sachet film ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,x,scfl}^{Hxl}$ = Hexanal concentration in gas phase which is in equilibrium with the sachet film material at a position x (x_{scfl}) ($\text{mol}\cdot\text{m}^{-3}$)
- C_{pkhs}^i = Concentration of active agent i in package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- C_{scfl}^i = Concentration of active agent i in sachet film ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{g,bed}^i$ = Equilibrium concentration of active agent i above the carrier bed ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{s,bed}^i$ = Equilibrium adsorbed amount of active agent i on the carrier bed ($\text{mol}\cdot\text{g}^{-1}$)
- $C_{s,bed,ini}^i$ = Initial value of equilibrium adsorbed amount of active agent i on the carrier bed ($\text{mol}\cdot\text{g}^{-1}$)
- $C_{pkhs,ini}^i$ = Initial value of concentration of active agent i in package headspace ($\text{mol}\cdot\text{m}^{-3}$)
- C_{pkfl}^i = Concentration of active agent i in packaging film ($\text{mol}\cdot\text{m}^{-3}$)
- $C_{pkfl,0}^i$ = Concentration of active agent i in packaging film at $x_{pkfl} = 0$

- $C_{pkfl, L_{pkfl}}^i$ = Concentration of active agent i in packaging film at $x_{pkfl} = L_{pkfl}$
 C_{env}^i = Concentration of active agent i in surrounding environment ($\text{mol}\cdot\text{m}^{-3}$)
 C_{sat}^{MCP} = 1-MCP saturated vapour concentration ($\text{mol}\cdot\text{m}^{-3}$)
 C_{scfl}^{MCP} = 1-MCP concentration in sachet film ($\text{mol}\cdot\text{m}^{-3}$)
 C_{pkfl}^{MCP} = 1-MCP concentration in packaging film ($\text{mol}\cdot\text{m}^{-3}$)
 C_{env}^{MCP} = 1-MCP concentration in environment ($\text{mol}\cdot\text{m}^{-3}$)
 $C_{scfl, 0}^{Hxl}$ = Hexanal concentration in sachet film at position $x_{scfl} = 0$ ($\text{mol}\cdot\text{m}^{-3}$)
 C_{sat}^{Hxl} = Saturated hexanal vapour concentration ($\text{mol}\cdot\text{m}^{-3}$) (i.e. $0.46 \text{ mol}\cdot\text{m}^{-3}$, at 20°C)
 $C_{g, pkfl, ini}^{Hxl}$ = Initial equilibrium concentration of hexanal vapour in packaging film ($\text{mol}\cdot\text{m}^{-3}$)
 $C_{g, pkfl, avg}^{Hxl}$ = Mean equilibrium concentration of hexanal vapour in film ($\text{mol}\cdot\text{m}^{-3}$)
 D = Mass diffusivity ($\text{m}^2\cdot\text{s}^{-1}$)
 D_{scfl}^{Hxl} = Hexanal mass diffusivity in the sachet film ($\text{m}^2\cdot\text{s}^{-1}$)
 d = Integration constant ($\text{mol}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$)
 D_{film}^i = Diffusivity of diffusant i in film ($\text{m}^2\cdot\text{s}^{-1}$)
 D_{scfl}^i = Mass diffusivity of active agent i in sachet film ($\text{m}^2\cdot\text{s}^{-1}$)
 D_{pkfl}^i = Mass diffusivity of active agent i in packaging film ($\text{m}^2\cdot\text{s}^{-1}$)
 $D_{fr}^{SO_2}$ = Effective mass diffusivity of SO_2 dissolved in fruit ($\text{m}^2\cdot\text{s}^{-1}$)
 D_{scfl}^{MCP} = Mass diffusivity of 1-MCP in sachet film ($\text{m}^2\cdot\text{s}^{-1}$)
 D_{pkfl}^{MCP} = Mass diffusivity of 1-MCP in packaging film ($\text{m}^2\cdot\text{s}^{-1}$)
 Ea = Energy of activation ($\text{J}\cdot\text{mol}^{-1}$)
 F_0 = Fourier number (dimensionless)
 ΔG° = Free energy ($\text{J}\cdot\text{mol}^{-1}$)
 ΔH_s = Heat of solution for the permeant gas ($\text{J}\cdot\text{mol}^{-1}$)
 ΔH° = Apparent enthalpy change ($\text{J}\cdot\text{mol}^{-1}$)
 J_{film} = Steady-state flux across film ($\text{mol}\cdot\text{s}^{-1}\cdot\text{m}^{-2}$)
 J_{film}^i = Steady-state diffusion flux of diffusant i in film ($\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$)

| | | |
|-----------------------|---|--|
| J_{scfl} | = | Steady-state flux at sachet boundary ($\text{mol}\cdot\text{s}^{-1}\cdot\text{m}^{-2}$) |
| K_{Lin}^i | = | Linear isotherm constant or partition coefficient of adsorbate i ($\text{m}^3\cdot\text{g}^{-1}$) |
| K_{Frd}^i | = | Freundlich constant ($\text{mol}^{1-n_{Frd}}\cdot\text{m}^{3n_{Frd}}\cdot\text{g}^{-1}$) |
| $K_{paper/air}$ | = | Partition coefficient ($\text{m}^3\cdot\text{g}^{-1}$) |
| $k_{tom, reac}^{Hxl}$ | = | Coefficient of reaction rate of hexanal and tomatoes ($\mu\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}\cdot(\text{m}^3\cdot\text{mol}^{-1})^{n_{reac}}$) |
| k | = | Surface mass transfer coefficient ($\text{m}\cdot\text{s}^{-1}$) |
| K_{bed}^i | = | Coefficient of the linear desorption isotherm of active agent i for the carrier (adsorbent) bed ($\text{m}^3\cdot\text{g}^{-1}$) |
| K_{bed}^{MCP} | = | Coefficient of linear sorption isotherm of 1-MCP for silica gel as reported by Lee (2003) ($\text{m}^3\cdot\text{g}^{-1}$) |
| $k_{fr}^{O_2}$ | = | Fruit skin permeance to gas O_2 ($\text{m}\cdot\text{s}^{-1}$) |
| $k_{fr, reac}^i$ | = | Rate coefficient for the reaction of the active agent i and fruit ($\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}(\text{m}^3\cdot\text{mol}^{-1})^{n_{reac}}$) |
| k_{mO_2} | = | Michaelis-Menten constant for O_2 consumption (kPa) |
| K_{Lin}^{Hxl} | = | Coefficient of the hexanal linear isotherm equation ($\text{g}\cdot\text{g}^{-1}$) |
| K_{GC}^i | = | Detector response or slope ($\text{mol}\cdot\text{area}^{-1}$) of standard curve of VOC i as shown in Figure C-1 |
| $k_{Lgmfl, 1}^{Hxl}$ | = | Coefficient of Langmuir relationship between hexanal vapour and LDPE film sorption ($\text{m}^3\cdot\text{mol}^{-1}$) |
| $k_{Lgmfl, 2}^{Hxl}$ | = | Coefficient of Langmuir relationship between hexanal vapour and LDPE film sorption (dimensionless) |
| k_{scfl} | = | Constant in simplified ODE (s^{-1}) |
| L_{film} | = | Film thickness (m) |
| L_{scfl} | = | Sachet film material thickness (m) |
| L_{pkfl} | = | Packaging film material thickness (m) |
| L | = | Characteristic dimension of bag (m) |
| li | = | Log integral function |
| M_{tom} | = | Mass of tomatoes (kg) |
| M_{bed} | = | Mass of the carrier bed (free of the mass of active agent i) (g) |
| m | = | Term in series solution (given as 5 terms) |

- N_{film}^i = Steady-state rate of transfer of gas i across the film ($\text{mol}\cdot\text{s}^{-1}$)
- n_{Frd} = Exponential factor ($0 < n_{Frd} < 1$) in Freundlich equation (dimensionless)
- n_{reac} = Order of reaction rate (dimensionless)
- $N_{fr}^{O_2}$ = Steady-state rate of transfer of gas O_2 across fruit skin ($\text{mol}\cdot\text{s}^{-1}$)
- $n_{pkhs}^{O_2}$ = Number of oxygen moles in package headspace (mol)
- $n_{pkhs}^{CO_2}$ = Number of carbon dioxide moles in package headspace (mol)
- ΔP_{film}^i = Partial pressure differential of gas i at both sides of film surfaces (Pa)
- P_{film}^i = Permeability to permeant i of the film ($\text{mol}\cdot\text{m}\cdot\text{s}^{-1}\cdot\text{m}^{-2}\cdot\text{Pa}^{-1}$)
- $P_{film,0}^i$ = Fitted pre-exponential factor for permeability to permeant i of the film ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- P_{film}^{Hxl} = Effective film permeability to hexanal ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{film,0}^{Hxl}$ = Fitted pre-exponential factor for effective permeability to hexanal of the film ($\text{pmol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{Tyvek,0}^{Hxl}$ = Fitted pre-exponential factor for effective permeability to hexanal of Tyvek[®], LDPE and OPP films, respectively ($\text{pmol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{LDPE,0}^{Hxl}$
- $P_{OPP,0}^{Hxl}$
- $P_{scfl,0}^{Hxl}$ = Pre-exponential factor of effective permeability to hexanal vapour of sachet film material ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{pkfl,0}^{Hxl}$ = Fitted pre-exponential factor for effective permeability to hexanal vapour of packaging film material ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{pkfl}^{O_2}$ = Film permeability to O_2 ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $P_{pkfl}^{CO_2}$ = Film permeability to CO_2 ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)
- $p_{pkhs}^{O_2}$ = O_2 partial pressure in the package headspace (kPa)
- $p_{env}^{O_2}$ = O_2 partial pressure in the bulk environment (kPa)
- $p_{env}^{CO_2}$ = CO_2 partial pressure in the bulk environment (kPa)
- $p_{pkhs}^{CO_2}$ = CO_2 partial pressure in the package headspace (kPa)
- P_{scfl}^i = Permeability to active agent i of sachet film material ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$)

| | | |
|--------------------|---|---|
| P_{pkfl}^i | = | Permeability to active agent i of packaging film material ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$) |
| P_{scfl}^{MCP} | = | Sachet film permeability to 1-MCP vapour ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$) |
| P_{pkfl}^{MCP} | = | Packaging film permeability to 1-MCP vapour ($\text{mol}\cdot\text{m}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$) |
| P_{pkfl}^{Hxl} | = | Permeability to hexanal vapour of the packaging film ($\text{m}^2\cdot\text{s}^{-1}$) |
| Q_{outlet} | = | Outgoing flowrate ($\text{m}^3\cdot\text{s}^{-1}$) |
| $Q_{l,conc}^{out}$ | = | Outlet gas flowrate from the low hexanal concentration side of the film ($\text{m}^3\cdot\text{s}^{-1}$) |
| R | = | Gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) |
| r_{tom}^{Hxl} | = | Apparent rates of uptakes of hexanal vapour by tomatoes ($\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}$) |
| r_{scfl} | = | Rate of changes of active agent concentration in the sachet film (dimensionless) |
| r_{bed} | = | Rate of changes of active agent concentration in carrier bed (dimensionless) |
| r_{pkhs} | = | Rate of changes of active agent concentration in package headspace (dimensionless) |
| r_{pkfl} | = | Rate of changes of active agent concentration in the packaging film (dimensionless) |
| $r_{fr}^{SO_2}$ | = | Reaction rate of SO_2 and corn ($\text{mol}\cdot\text{m}^{-3}\cdot\text{s}^{-1}$) which Haros et al. (2005) assumed to follow first order kinetics |
| R_{fr} | = | Radius of fruit (assumed to be spherical) (m) |
| r_{fr}^i | = | Reaction rate of between active agent i and fruit ($\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}$) |
| r_{pkhs}^i | = | Rate of accumulation of active agent i in package headspace ($\text{mol}\cdot\text{s}^{-1}$) |
| r_{scfl}^{Hxl} | = | Rate of hexanal permeation through the sachet film material ($\text{mol}\cdot\text{s}^{-1}$) |
| r_{pkfl}^{Hxl} | = | Rate of hexanal permeation through the packaging film material ($\text{mol}\cdot\text{s}^{-1}$) |
| r_{O_2} | = | Rate of O_2 consumption by respiration ($\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}$) |
| $r_{O_2}^{max}$ | = | Maximum O_2 consumption rate ($\text{mol}\cdot\text{kg}^{-1}\cdot\text{s}^{-1}$) |
| r_{CO_2} | = | Rate of respiratory CO_2 production ($\text{mol}\cdot\text{s}^{-1}\cdot\text{kg}^{-1}$) |
| R_{pkfl} | = | Half thickness of film (m) |

| | |
|-------------------|---|
| S_{film}^i | = Solubility coefficient of gas i into film ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| $S_{film,0}^i$ | = Fitted pre-exponential factor for solubility to permeant i of the film ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| ΔS° | = Entropy ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) |
| S_{scfl}^i | = Sachet film solubility to active agent i ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{scfl}^{MCP} | = Sachet film solubility to 1-MCP as reported by Lee (2003) ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{pkfl}^i | = Packaging film solubility to active agent i ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{scfl}^{Hxl} | = Sachet film solubility to hexanal ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{scfl}^{MCP} | = Sachet film solubility to 1-MCP ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{pkfl}^{MCP} | = Packaging film solubility to 1-MCP ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| S_{pkfl}^{Hxl} | = Packaging film solubility to hexanal vapour ($\text{mol}\cdot\text{m}^{-3}\cdot\text{Pa}^{-1}$) |
| T_{film} | = Measured film temperatures (K) |
| $T_{10^\circ C}$ | = Temperature (K) for 10 and 20°C, respectively |
| $T_{20^\circ C}$ | |
| T_{pkg} | = Temperature of package (K) |
| t | = Time (s) |
| V_{pkg} | = Volume of package (m^3) |
| Vol_{inj} | = Injected volume of sample (m^3) |
| x_{film} | = Position in film (m) |
| x_{fr} | = Position in fruit (m) |
| x_{pkfl} | = Position in packaging film material (m) |
| x_{scfl} | = Position in sachet film (m) |
| Y_{avg} | = Fraction unaccomplished change of concentration (dimensionless) |
| Z_{Lgmfl}^{Hxl} | = Fitted coefficient of Langmuir relationship for hexanal vapour sorption on LDPE film ($\text{mol}\cdot\text{s}^{-1}\cdot\text{m}^{-2}$) |

LIST OF FIGURES

- Figure 2-1 Brunauer's five types of adsorption isotherm of which V_{ads} , p , p^0 and B representing sorption extents (volume), pressure, saturated pressure, and a knee of the curve indicating a completion of a monolayer (reprinted from Adamson 1990).....2-14
- Figure 2-2 Adsorption isotherm of 1-MCP on silica gel at 50, 60, 70, and 80°C (digitally redrawn from Lee 2003); lines representing the Linear adsorption isotherm model (Eq. 2-2).2-15
- Figure 2-3 Mass transport steps during adsorption by a porous adsorbent (redrawn after Weber 1985).....2-19
- Figure 3-1 Hexanal exposure system comprising with 2 key compartments: an exposure chamber (a 5 L glass desiccators) and the 250 ml glass bubbling tubes.....3-4
- Figure 3-2 Hexanal concentrations during the continuous exposure period (3 replicates shown for each sampling time)3-8
- Figure 3-3 Tomatoes kept under different gas compositions: 40-70 ppm, at day 7 (A), 5-15 ppm on day 2 and day 4, respectively (B and C), and day 2 after leaving 40-160 ppm treated tomatoes in the ambient condition (D).....3-9
- Figure 3-4 Respiration (RR), ethylene production (EP), and hue angle (Hue) of tomatoes exposed to hexanal vapour through continuous (40-70 ppm) (A) or single dose (200-270 ppm) (B) delivery systems. The symbols (\diamond), (\circ), and (\blacksquare) represent average results (10 replicates) obtained from day 0, hexanal-treated tomatoes, and control treatments, respectively. Error bars at day 0 represent standard deviation from the mean. Hexanal concentrations in the exposure chamber during the storage period were represented by the symbol (+) in the RR-A graph (3 replicates shown for each sampling time)3-11
- Figure 3-5 Comparison of skin colours after 7 days storage of tomatoes kept in hexanal-free air (top row) or continuously exposed to hexanal (bottom row)3-13
- Figure 3-6 Effects of temperature and concentration on apparent uptake rates of hexanal by tomatoes at 10 and 20°C (3 replicates for individual treatments shown for each sampling time). Solid lines were fitted by nonlinear regression using Eq. 3-2; referred to Table 3-4 for model coefficients.3-16
- Figure 3-7 Hexanal consumption rates by sliced 'Golden Delicious' apples, at 5-23°C (redrawn from Wolford 1998), and their comparisons to apparent uptake rates by tomatoes measured in the present work3-19

- Figure 3-8 Effects of modified atmosphere conditions on apparent hexanal uptake rates of tomatoes (3 replicates for individual treatments shown for each sampling time)..... 3-23
- Figure 3-9 Inlet and outlet hexanal concentrations measured during experiments on the effects of modified atmosphere (MA) conditions on apparent hexanal uptake rates of tomatoes (3 replicates for individual treatments shown for each sampling time)..... 3-24
- Figure 3-10 Respiration rates of tomatoes at 20°C measured at different treatments (3 replicates of individual treatments shown for each sampling time)..... 3-25
- Figure 4-1 Experimental set-up for measurement of film permeability to hexanal vapour (A) and cross section of stainless steel permeability cell (B) (modified from Merts 1996) 4-4
- Figure 4-2 Effective permeability to hexanal of Tyvek[®] (A), LDPE (B) and OPP (C) measured at 10 and 20°C. (Three replicates are shown for each concentration difference tested). The solid lines were fitted using nonlinear regression (Eq. 4-3). Note a different y-axis scale was chosen for each graph to better represent the data. 4-8
- Figure 4-3 Steady-state concentration gradients predicted using Eq. 4-4 for conditions when large (as a case of OPP film; dashed and dashed-dotted line) and small and moderate (as a case of LDPE film; solid and dotted lines, respectively) concentration gradients. On the x-axis, $x=0$ represents the film surface facing the high hexanal concentration ($C_{h,conc}^{Hxl}$) and $x=1$ the film surface facing against the low concentration ($C_{l,conc}^{Hxl}$). 4-12
- Figure 4-4 Comparison of sorption isotherms for ethanol and acetaldehyde measured using the gravimetric sorption method used for silica gel adsorbents for experimental (■) and literature data (o) reported for ethanol by Madeley & Sing (1959) (A) and acetaldehyde by Ghosh & Hines (1990) (B). Experimental data were collected at the same temperatures as the reported data, namely 25°C for ethanol and 14°C for acetaldehyde. 4-28
- Figure 4-5 Hexanal sorption isotherms for silica gel grade 40 at 10 and 20°C measured using a gravimetric sorption approach. Solid lines were fitted using the Langmuir isotherm model Eq. 2-3. 4-29
- Figure 5-1 Mass transfer processes for release of volatiles gaseous components in an active MAP system with enclosed sachet and a horticultural product (subscripts: $pkhs$, $pkfl$, $scfl$ env and fr represent package headspace, packaging film, sachet film, environment

| | |
|--|------|
| and fruit, respectively; superscript i represents active agent i ; MA and RH represent modified atmosphere and relative humidity, respectively)..... | 5-2 |
| Figure 5-2 Conceptualisations of internal and external resistances of an entire bed of porous particles encasing in the sachet (A) and individual particles (B; modified from Weber 1985; Do 1998a where ‘ λ ’ and ‘ d ’ symbols represent active agent in the gas phase and diameter of pore inside the particle, respectively). | 5-9 |
| Figure 5-3 Conceptualisation of diffusional modes within the bed (given negligible concentration gradient within particles): Particle surface diffusion, where the magenta rings represent thin films through which diffusion occur (A), and gas phase diffusion within voids available between particle (B)..... | 5-10 |
| Figure 5-4 Simulations of 1-MCP accumulation in the package headspace as predicted by steady-state and PDE (with the 1 st kind of boundary condition) models, represented by solid and dotted lines, respectively. $CR_{pkhs/scfl}$ was varied by changing S_{scfl}^{MCP} values. | 5-16 |
| Figure 5-5 Simulations of 1-MCP accumulation in the package headspace as predicted by steady-state and PDE (with the 1 st kind of boundary condition) models, represented by solid and dotted lines, respectively. $CR_{pkhs/pkfl}$ was varied by changing S_{pkfl}^{MCP} values. | 5-19 |
| Figure 5-6 A comprehensive decision tree for design of active packaging systems for horticultural products. The modelling options employed for hexanal based active MAP for tomatoes are identified by red lines (see over for nomenclatures)..... | 5-25 |
| Figure 5-7 Finite difference grid for packaging film..... | 5-33 |
| Figure 6-1 Examples of active MA package containing tomatoes (A) or a sealed glass container (B)..... | 6-2 |
| Figure 6-2 Effects of sachet gel loading on hexanal concentration in the headspace of package (C_{pkhs}^{Hxl}) containing an inert sealed glass jar, stored at 20°C. Experimental data (at least 3 replicates shown for each sampling time) of 1.5, 3.0 and 4.5 g loadings are represented by \circ , \diamond and $+$ symbols, respectively, for a storage period of 7 days (A), and for the same data expanded to look at the first 24 h (B). Model predictions for each gel mass are shown through solid, dotted and dashed lines, respectively. | 6-7 |
| Figure 6-3 Model predictions of hexanal partial relative pressures (p/p_s) in the package headspace (dashed line) and sachet headspace (dotted line), and the hexanal mass | |

- remaining on the silica gel (solid line) for the LD1 system (1.5 g dried silica gel; Table 6-1). 6-8
- Figure 6-4 Sachet headspace concentration ($C_{g,bed}^{Hxl}$) predicted for hexanal saturated initial dried silica gel masses of 1.5, 3.0 and 4.5 g (represented by solid, dotted and dashed lines, respectively). 6-9
- Figure 6-5 Changes in ethanol concentration in the atmosphere of perforated polyethylene bags packed with broccoli branchets (digitally redrawn from Suzuki et al. 2004) (A), or above a_w -adjusted PDA plates, packaged with Ethicap[®] type E₁ and E₄ in high ethanol barrier pouch (digitally redrawn from Smith et al. 1987; note data on day 7th of E₄ + a_w 0.85 was not reported) (B). 6-11
- Figure 6-6 Effects of sachet loading on hexanal accumulation in the headspace of package containing tomatoes kept at 20°C. Experimental data (at least 3 replicates shown for each sampling time) for loadings of 1.5, 3.0 and 4.5 g are shown in (A), (B) and (C), respectively, where headspace hexanal concentrations of packages containing either a sealed jar (○; as previously reported) or and tomatoes (◇) are compared, for which prediction results were represented by solid and dotted lines, respectively. 6-17
- Figure 6-7 Simulations of hexanal mass remaining on silica gel due to hexanal release from the sachet to the package headspace (LHS y-axis) and the hexanal mass transferred through the packaging film or taken up by tomatoes (RHS y-axis). All simulations were based on LD1 active packaging system containing tomatoes and 1.5g dried silica gel as the hexanal carrier (Table 6-1). 6-19
- Figure 6-8 Measured and predicted headspace gas at 20°C (2 replicates shown for each sampling time) measured in active (○ and ●, for O₂ and CO₂, respectively) and passive (◇ and ◆, for O₂ and CO₂, respectively) MA packages. The dotted and dashed lines are the MA model predictions. 6-20
- Figure 6-9 Measured and predicted hexanal concentration in the active package (at least 3 replicates shown for each sampling time), for different ratios of sachet to bag area (ω_A): 0.024 (○; LD1), 0.012 (◇; LD5), and 0.048 (+; LD6), for storage period of 7 days at 20°C (A) and the same data expanded to look at the first 24 h (B). Model predictions are shown through solid, dotted and dashed lines, respectively. 6-23
- Figure 6-10 Effects of OPP sachet film on package headspace hexanal concentration (at least 3 replicates shown for each sampling time) in a LDPE package containing either a

- sealed glass jar (○) or tomatoes (◇) of which prediction results are represented by solid and dotted lines, respectively.6-24
- Figure 6-11 Effects of Tyvek® sachet film on hexanal accumulation in the headspace of an LDPE package (at least 3 replicates shown for each sampling time) containing either a sealed glass jar (○) or tomatoes (◇) of which model prediction results are represented by solid and dotted lines, respectively.6-26
- Figure 6-12 Results of sensitivity analyses of Tyvek®-sachet model package containing a sealed glass jar, by simultaneously varying values of b_{Lgm}^{Hxl} and a combination of L_{pkfl} and P_{LDPE}^{Hxl} to change equilibrium sorption characteristics and film permeance, respectively. Experimental results are represented by black symbols (at least 3 replicates shown for each sampling time). The solid line represents model predictions using the original model inputs (A). Model inputs were varied to either minimise (by increasing sorption affinity and outer film permeance) (B) or maximise (by lowering sorption affinity and outer film permeance) (C) accumulation of hexanal vapour and these model predictions are represented by the dotted and dashed lines, respectively.6-29
- Figure 6-13 Hexanal concentrations in model packages (at least 3 replicates of individual treatments shown for each sampling time) with LDPE, OPP and Tyvek® as the sachet film material, at variable 10°C and 20°C storage conditions. Experimentally collected data for packages containing either a sealed jar (○), or tomatoes (◇) is presented in the first column (A; suffix ‘all’). Individual sets (B, and C; suffix ‘jar’ and ‘tom’ representing sealed jars and tomatoes, respectively) are presented with model predictions, where solid and dotted lines describe the predicted results at 10°C and 20°C, respectively. The transitions between 10 and 20°C occurred at day 7 (10 to 20°C) and day 12 (20 to 10°C) as shown in A (top).6-30
- Figure 6-14 Sorption isotherm at 10 and 20°C (calculated using the Langmuir Equation; (Eq. 2-3) and coefficients reported in Table 4-9). The letters A, B (and B’), C, and D represent those points discussed in the text regarding changes to the sorption equilibrium during temperature transitions.6-32
- Figure 6-15 Experimental and predicted values of hexanal concentration in an LDPE-sachet package containing a sealed glass jar (at least 3 replicates shown for each sampling time) during varied storage temperature regimes. Solid and dotted lines represent model predictions on 10 and 20 °C (A). Hexanal sorption isotherms at 10 and 20°C were calculated using the Langmuir equation (Eq. 2-3 and coefficients reported in

- Table 4-9) (labelled as ‘original’), and the isotherm at 20°C when $C_{s,max}^{Hxl}$ value was arbitrarily assumed to be the value at 10°C, with the b_{Lgm}^{Hxl} value as at 20°C (B). 6-35
- Figure 6-16 Results of sensitivity analyses of model package at 10°C containing a sealed glass jar (at least 3 replicates shown for each sampling time), by simultaneously lowering outer film permeance (by decreasing P_{LDPE}^{Hxl} and increasing L_{pkfl}) and sorption affinity (by lowering b_{Lgm}^{Hxl}). 6-37
- Figure 6-17 Experimental data on changes of adsorbed hexanal mass on silica gel (○) and model prediction (solid line) with an adjusted model prediction to correct for initial free liquid mass. 6-39
- Figure 6-18 Comparisons of fluxes measured in experiments on LDPE film permeability (section 4.2.2) and hexanal mass loss (this section) to fluxes predicted by (i) Eq. 4-5 (section 4.2.2; □) or Eq. 6-3 (Δ), and flux calculated from results of hexanal mass loss (○). The dotted line represents $y = x$ line. 6-42
- Figure 6-19 Experimental data on changes of adsorbed hexanal mass on silica gel (○) and model prediction (solid line) using Eq. 6-3. 6-44
- Figure 6-20 Experimental data (○; at least 3 replicates shown for each sampling time) on hexanal vapour concentrations in package headspace of LD1 active packaging system (with no tomatoes; Table 6-1) and model prediction results of original (solid line) and modified (dotted line) global mathematical model, during 7-day (A) and 24-hour storage period (B; the same data expanded to better present). 6-45
- Figure 7-1 Conceptualised release patterns to extend shelf life (SL_0 and SL_{AP} represent the shelf life without and with active controlled release, respectively) and delay changes of postharvest qualities (dotted lines). Solid lines represent long (I) and short (II) sustained release period prior to concentration decreasing, while the solid line III represents the fumigation with a high concentration following by an attainment of a low concentration. 7-2
- Figure 7-2 Alternative sorption isotherm shapes for simulating hexanal release patterns. Coefficients associated with the isotherm equations are those shown in Table 7-1. 7-4
- Figure 7-3 Simulated hexanal release patterns for alternative hexanal sorption isotherms: Exponential (Exp.1-3, represented by solid, dotted and dashed lines, respectively), Linear (Lin.), and Langmuir (Lgm.1-3, represented by solid, dotted and dashed lines, respectively). Graphs on the left- and right-hand-side columns refer to active MA

packages having LDPE and OPP respectively as outer film materials, with the same sorption isotherm systems shown on the same row. Legends shown in these graphs (on the left-hand-side (LHS) column) refer to the parameter sets as provided in Table 7-1.

-7-6
- Figure 7-4 Simulated hexanal release patterns for alternative hexanal sorption isotherms with 10-fold lower outer bag permeability: Exponential (Exp.1-3 represented by solid, dotted and dashed lines, respectively), Linear (Lin.), and Langmuir (Lgm.1-3 represented by solid, dotted and dashed lines, respectively) and legends shown in these graphs (on LHS column) refer to variations as provided in Table 7-1. Graphs on the right-hand-side (RHS) column show sachet headspace concentrations and lines refer to sorption isotherm systems as provided in the same row of the LHS column.7-8
- Figure 7-5 Simulation results demonstrating the influences of PAR values on package headspace quasi steady-state concentrations of hexanal vapour (on day 7; at 20°C) in LD1 active MAP systems (without tomatoes) for Exponential (Exp.1) Linear (Lin.), and Langmuir (Lgm.1) isotherms (represented by dashed dotted and solid lines, respectively; refer to Table 7-1) (A) and release profiles considered at $PAR = 0.8$ (B).
.....7-10
- Figure 7-6 Mathematical model simulations of MA conditions at 20°C in hexanal active MA package containing 6 medium tomatoes (~600g) having either LDPE or OPP films as outer packaging films. See text for conditions.7-13
- Figure 7-7 Simulated fluxes across the sachet boundary as a function of $C_{s,bed}^{Hxl}$, according to selected Exponential (Exp.1), Linear (Lin.) and Langmuir (Lgm.1) isotherm models (represented by dashed dotted and solid lines, respectively; refer to Table 7-1).7-16
- Figure 7-8 Simulated fluxes across the sachet boundary for the exponential (Exp.1), linear (Lin.) and Langmuir (Lgm.1) sorption isotherms, respectively. The coefficients of the isotherm models are those shown in Table 7-1.7-18
- Figure 7-9 Ethanol sorption isotherms for Ajax activated carbon at 25°C (Prasetyo et al. 2002) (A), silica gel at 25°C (Madeley & Sing 1959) (B), and Amorphous Teflon AF2400 at 30°C (Tokarev et al. 2006) (C). All isotherm data were digitally redrawn using the TechDig software. Dotted, solid and dashed lines represent ethanol equilibrium sorptions predicted by the Freundlich (Eq. 2-4), Langmuir (Eq. 2-3) and exponential (Eq. 7-3) models, respectively.7-20
- Figure 7-10 Ethanol vapour concentrations released from 4 ml_{EtOH}/kg_{fruit} (●) and 8 ml_{EtOH}/kg_{fruit} (◊) loading ratios of liquid ethanol saturated paper (RHS y-axis) as

| | |
|---|------|
| reported by Lurie et al. (2006) and data were digitally redrawn using the TechDig software. Solid and dotted lines represent model predictions of the Langmuir ethanol sorption isotherm for silica gel, provided model in puts in Table 7-4. See text for simulation conditions (for Sim.1 and Sim.2). | 7-22 |
| Figure 7-11 Simulated results of influences of PAR values on package headspace quasi steady-state concentrations of ethanol vapour (on day 7) in LD1 active MAP systems having different sorption isotherms which are Freundlich, Langmuir and exponential isotherms for activated carbon (A), silica gel (B) and Teflon (C) systems, respectively. | 7-24 |
| Figure C-1 Standard curves of hexanal, acetaldehyde, and ethanol (n^i = number of moles) | C-2 |
| Figure E-1 Hexanal sorption isotherm for silica gel at 20°C (3 replicates shown for each uptake) quantified by the Pulse IGC technique..... | E-3 |
| Figure E-2 Comparison of hexanal uptake by silica gel grade 40 at 20°C, quantified by FIGC method (○) and gravimetric method (■; reported in Chapter 4) | E-4 |
| Figure E-3 Comparison of acetaldehyde uptake by silica gel grade 40 at 14°C, quantified by the FIGC method (○) and gravimetric method (■; as reported by Ghosh & Hines 1990)..... | E-6 |
| Figure E-4 Comparison of hexanal uptake by silica gel grade 40 at 20°C quantified by the gravimetric method (as reported in Chapter 4) and by the volumetric method at 10 and 20°C | E-7 |
| Figure E-5 Predictions of hexanal concentration in package headspace (A) and equilibrium hexanal vapour in sachet headspace (B) in a model active package (without packaged tomatoes), kept at 20°C during 7 days, using Langmuir model coefficients which were obtained from gravimetric (solid line) and the volumetric (Autosorb-1 instrument; dotted line) sorption isotherms. | E-10 |
| Figure E-6 Plots of $(p/p_s)/C_{s,bed}^{Hxl}$ against p/p_s for hexanal sorption isotherm data at 10 and 20°C for estimating Langmuir equation coefficients according to the reparameterisation approach proposed by Ratkowsky (1990) | E-12 |
| Figure E-7 Hexanal sorption isotherms for silica gel grade 40 at 10 and 20°C, measured using a gravimetric sorption approach and presented in molar units. Solid lines were fitted using Langmuir isotherm model (Eq. 2-3)..... | E-13 |
| Figure F-1 Conceptual model of one-dimensional mass transfer across a sachet film..... | F-2 |

| | |
|--|------|
| Figure F-2 Conceptual model of the concentration gradient of volatile across the sachet film | F-5 |
| Figure F-3 Conceptual model of mass transfer across packaging film in an active packaging system | F-11 |
| Figure F-4 Conceptual model of the initial concentration gradient of 1-MCP across the packaging film..... | F-12 |
| Figure G-1 Comparison of mean concentrations of equilibrium hexanal vapour in the packaging film from analytical ($m = 5$) and numerical solutions for diffusion mass transfer with the first kind of boundary condition. | G-9 |
| Figure G-2 Comparison of the numerical and analytical solutions for package headspace hexanal concentration, of which hexanal mass transfer across sachet film was modelled using steady-state approach..... | G-11 |

LIST OF TABLES

| | |
|---|------|
| Table 2-1 Comparison of different controlled release active packaging configurations (modified from Rooney 1995a; Smith et al. 1995; Han 2000; Han 2003)..... | 2-12 |
| Table 2-2 A summary of active MAP systems that can release active agents into the package headspace and their reported application for horticultural products..... | 2-13 |
| Table 2-3 Shapes and fitted equations of sorption isotherms for selected certain active agents for silica gel adsorbents ^a | 2-16 |
| Table 2-4 Mechanisms and characteristics of intraparticle transport models (Geankoplis 1993b; Do 1998a; Johnson 1999; Mugge et al. 2001) | 2-20 |
| Table 2-5 Selected works using Fick's second law to model diffusion of active agents in polymeric materials, for controlled release applications. | 2-23 |
| Table 3-1 Description of working example MAP system: an Active MAP with a hexanal vapour controlled release sachet for tomatoes | 3-1 |
| Table 3-2 Effect of continuous and single-dose hexanal vapour exposure on growth of <i>Botrytis cinerea</i> on wound-inoculated tomatoes. The percentages of fruit exhibiting fungal growth are represented by the symbols: -, +, ++, +++, +++++. These symbols represent 0, 10-30, 40-60, 70-90 and 100% of fruit infected, respectively..... | 3-8 |
| Table 3-3 Comparison of postharvest physiology and quality attributes of tomatoes between data of the present work (cv. 'Royale'; measured at 20°C) and those of estimates from previously published data | 3-14 |
| Table 3-4 Parameter estimates and standard errors (SE) ^a resulting from nonlinear regression analysis of hexanal consumption rates by tomatoes at 10 and 20°C | 3-18 |
| Table 3-5 Gas streams introduced to the exposure chamber (as experimental treatments) | 3-22 |
| Table 4-1 Hexanal vapour concentrations and carrier gas flowrates delivered to the permeability cell..... | 4-5 |
| Table 4-2 Parameter estimates and standard errors (SE) resulting from nonlinear regression analysis of permeability to hexanal vapours of Tyvek [®] , LDPE, and OPP films, measured at 10 and 20°C..... | 4-10 |
| Table 4-3 Estimated permeability to various VOCs of Tyvek [®] building materials measured at 23°C (modified from Yang et al. 2005) ^a | 4-15 |
| Table 4-4 Comparison of permeability of OPP and PP films to hexanal and other selected volatile organic compounds (VOCs)..... | 4-17 |

| | |
|---|------|
| Table 4-5 Summary of T_g values of a range of polymer films for food packaging applications (modified from Brandsch & Piringer 2000; Willige et al. 2002; Selke et al. 2004)..... | 4-19 |
| Table 4-6 Comparison of permeability of LDPE and other polyethylene family films to hexanal and other selected volatile organic compounds (VOCs) | 4-21 |
| Table 4-7 General properties of silica gel grade 40 | 4-26 |
| Table 4-8 Parameter estimates and standard errors (SE) from nonlinear regression analysis of hexanal sorption isotherm data for silica gel grade 40 at 10 and 20°C | 4-31 |
| Table 4-9 Parameters of the Langmuir model equation estimated using nonlinear regression for literature data on sorption of a range of VOCs for silica gel adsorbents | 4-32 |
| Table 4-10 Apparent thermodynamic parameters for hexanal sorption onto silica gel adsorbents at 10 and 20°C | 4-34 |
| Table 4-11 Experimental results on the effects of RH on hexanal sorption isotherm for silica gel adsorbents | 4-35 |
| Table 5-1 Estimated B_i values for diffusion of certain active agents in the package headspace | 5-6 |
| Table 5-2 Internal and external resistances according to bed and particles in sachet systems | 5-9 |
| Table 5-3 Input data of 1-MCP active packaging system (at 23°C; following Lee 2003) for illustrating scaling analyses..... | 5-14 |
| Table 6-1 Details of the active MA packages employed in the validation trials (all used a LDPE outer bag)..... | 6-2 |
| Table 6-2 Summary of system inputs used for mathematical model validation..... | 6-4 |
| Table 6-3 Range of key model inputs and the justification of their use in sensitivity analyses | 6-5 |
| Table 6-4 Examples of model sensitivity to input variables for the system having a LDPE sachet with 4.5 g loading (LD3; Table 6-1). Experimental data are shown as \circ symbols. | 6-13 |
| Table 7-1 Coefficients associated with alternative isotherm equations..... | 7-4 |
| Table 7-2 Model inputs for simulating the effects of PAR on quasi steady-state concentrations of LD1 active MAP systems (without tomatoes) for Exponential (Exp.1) Linear (Lin.), and Langmuir (Lgm.1) isotherms (Table 7-1)..... | 7-11 |

| | |
|---|------|
| Table 7-3 Parameters of the Freundlich, and exponential model equations estimated using nonlinear regression for literature data on ethanol sorption for activated carbon and Teflon..... | 7-21 |
| Table 7-4 Key model inputs used for simulations of ethanol vapour releases | 7-23 |
| Table C-1 Gas chromatography conditions for identifying acetaldehyde and ethanol..... | C-1 |
| Table E-1 Parameter estimates and standard errors (SE) from nonlinear regression analysis of the hexanal sorption isotherm data at 20°C as measured by the volumetric-method | E-8 |
| Table E-2 Langmuir coefficients estimated using the reparameterisation proposed by Ratkowsky (1990) | E-12 |
| Table E-3 Parameter estimates and standard errors (SE) from nonlinear regression analysis of hexanal sorption isotherm data for silica gel grade 40 at 10 and 20°C (presented in molar units as illustrated in Figure E-7)..... | E-13 |
| Table F-1 Estimated B_i values for diffusion of hexanal in sachet and package atmosphere | F-1 |
| Table F-2 MATLAB® filenames for simulations of 1-MCP accumulation in package headspace | F-19 |
| Table F-3 Estimated values of $CR_{bed/scfl}$, $CR_{pkhs/scfl}$ and $CR_{pkhs/pkfl}$ for hexanal mass transfer in active packaging systems | F-20 |
| Table H-1 Examples of model sensitivity to input variables: 4.5 g LDPE sachet loading experiment of active packages containing tomatoes (experimental data shown as \diamond symbols), with discussion made in section 6.4.1.2. | H-2 |
| Table H-2 Examples of model sensitivity to input variables: MA condition of active packages containing tomatoes is the same as that employed in Table H-1 (experimental data of O_2 and CO_2 shown as \circ and \diamond symbols, respectively), with discussion made in section 6.4.1.2. Variations employed for varying values of $r_{O_2}^{max}$, k_{mO_2} , and permeability values (both $P_{pkfl}^{O_2}$ and $P_{pkfl}^{CO_2}$) are 10%, 20%, and 10%, respectively (as utilised by in Merts 1996; Tanner 1998). Variation of package volume is as shown in Table 6-3. | H-4 |
| Table H-3 Examples of model sensitivity to input variables: model package LD6 (experimental data shown as \circ symbols), with discussion made in section 6.4.2. | H-5 |
| Table H-4 Examples of model sensitivity to input variables: model package containing tomatoes and OPP film as a sachet film material (experimental data shown as \diamond symbols), with discussion made in section 6.4.3.1. | H-6 |

| | |
|--|-----|
| Table H-5 Examples of model sensitivity to input variables: model package containing tomatoes and Tyvek [®] film as a sachet film material (experimental data shown as \diamond symbols), with discussion made in section 6.4.3.2. | H-7 |
| Table H-6 Examples of model sensitivity to input variables: model package containing tomatoes kept at 10°C, sachet materials were LDPE, OPP, and Tyvek [®] (experimental data shown as \diamond symbol) ¹ , with discussion made in section 6.4.4..... | H-8 |
| Table H-7 Examples of model sensitivity to input variables: changes of hexanal amount on silica gel (empirical data shown as \circ symbols). Initial hexanal adsorbed amount used in the modified global model was referred to as the effective amount. Results for discussion are made in section 6.4.5. | H-9 |